Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1KYO
Title	:	YEAST CYTOCHROME BC1 COMPLEX WITH BOUND SUBSTRATE CYTOCHROME C
Authors	:	Lange, C.; Hunte, C.
Deposited on	:	2002-02-05
Resolution	:	2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

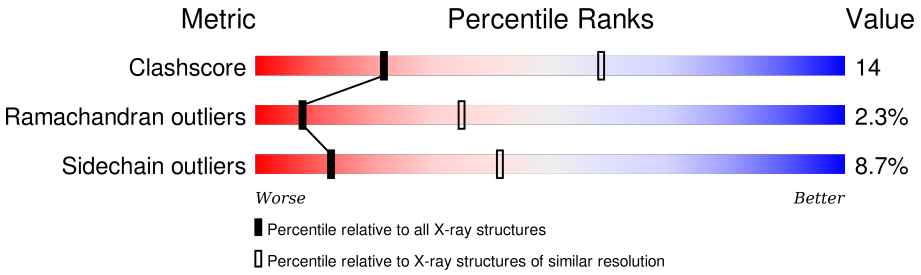
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	430	70% 26% •
1	L	430	65% 30% 5%
2	B	352	58% 36% 6% •
2	M	352	58% 35% 7% •
3	C	385	70% 27% •
3	N	385	73% 23% •
4	D	248	80% 17% ••

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Mol	Chain	Length	Quality of chain
4	O	248	75% 23%
5	E	185	69% 28%
5	P	185	75% 24%
6	F	74	70% 28%
6	Q	74	73% 24%
7	G	126	77% 21%
7	R	126	74% 23%
8	H	93	63% 30% 5%
8	S	93	66% 27% 6%
9	I	57	65% 26% 7%
9	T	57	74% 16% 7%
10	J	127	51% 38% 10%
10	U	127	50% 43% 7%
11	K	107	56% 36% 7%
11	V	107	56% 39% 5%
12	W	108	61% 31% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SMA	C	505	X	-	-	-
15	SMA	N	525	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 35643 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3338	2106	575	651	6			
1	L	430	Total	C	N	O	S	0	0	0
			3338	2106	575	651	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP P07256
A	152	ASP	GLU	CONFLICT	UNP P07256
L	?	-	SER	DELETION	UNP P07256
L	152	ASP	GLU	CONFLICT	UNP P07256

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			
2	M	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			
3	N	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	270	VAL	ASP	SEE REMARK 999	UNP P00163
N	270	VAL	ASP	SEE REMARK 999	UNP P00163

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1929	1229	332	359	9			
4	O	245	Total	C	N	O	S	0	0	0
			1929	1229	332	359	9			

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			
5	P	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			625	390	108	125	2			
6	Q	74	Total	C	N	O	S	0	0	0
			625	390	108	125	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	74	ASP	VAL	CONFLICT	UNP P00127
Q	74	ASP	VAL	CONFLICT	UNP P00127

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			
7	R	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			
8	S	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	53	Total	C	N	O	0	0	0
			436	292	71	73			
9	T	53	Total	C	N	O	0	0	0
			436	292	71	73			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	55	LYS	ARG	CONFLICT	UNP P22289
T	55	LYS	ARG	CONFLICT	UNP P22289

- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			
10	U	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			
11	V	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

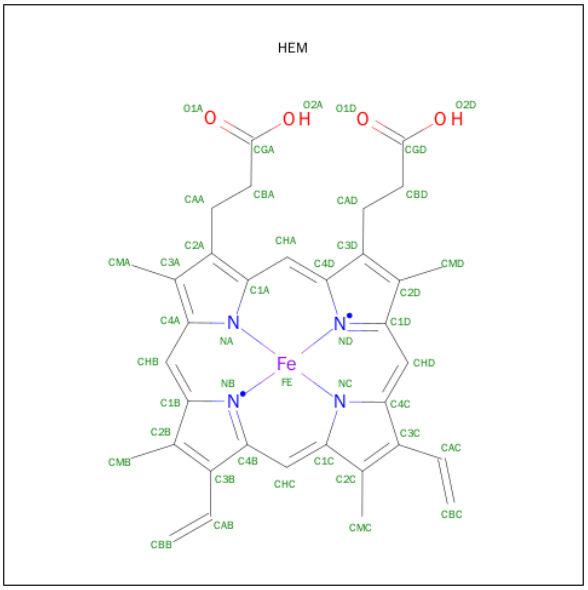
- Molecule 12 is a protein called CYTOCHROME C, ISO-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	0	0
			850	537	151	157	5			

There is a discrepancy between the modelled and reference sequences:

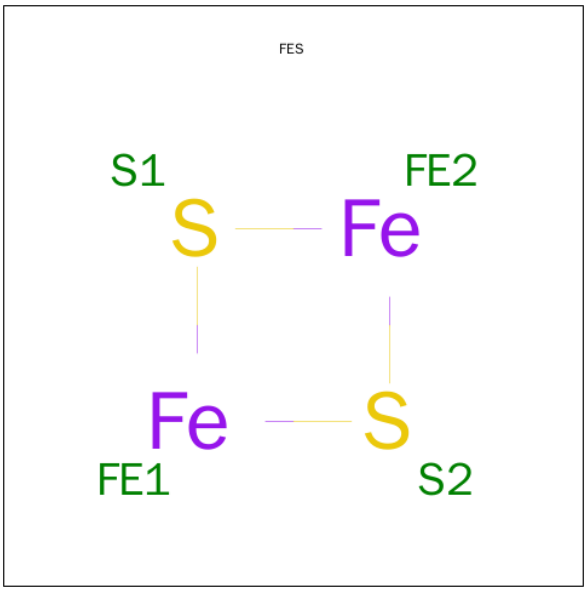
Chain	Residue	Modelled	Actual	Comment	Reference
W	77	M3L	LYS	MODIFIED RESIDUE	UNP P00044

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



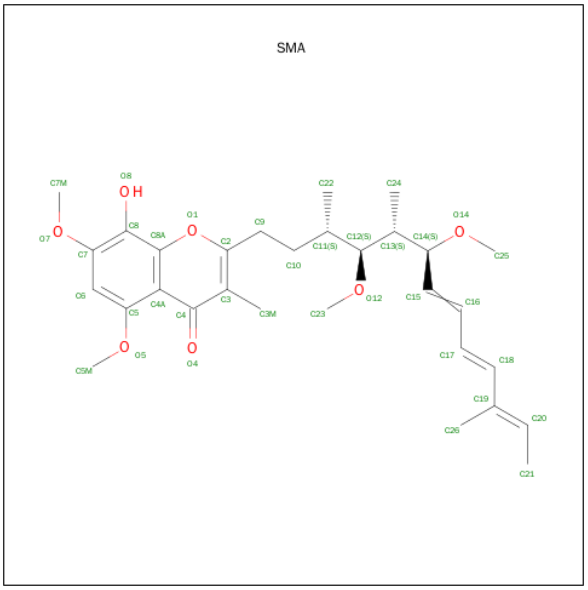
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	E	1	Total Fe S 4 2 2	0	0
14	P	1	Total Fe S 4 2 2	0	0

- Molecule 15 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C O 37 30 7	0	0
15	N	1	Total C O 37 30 7	0	0

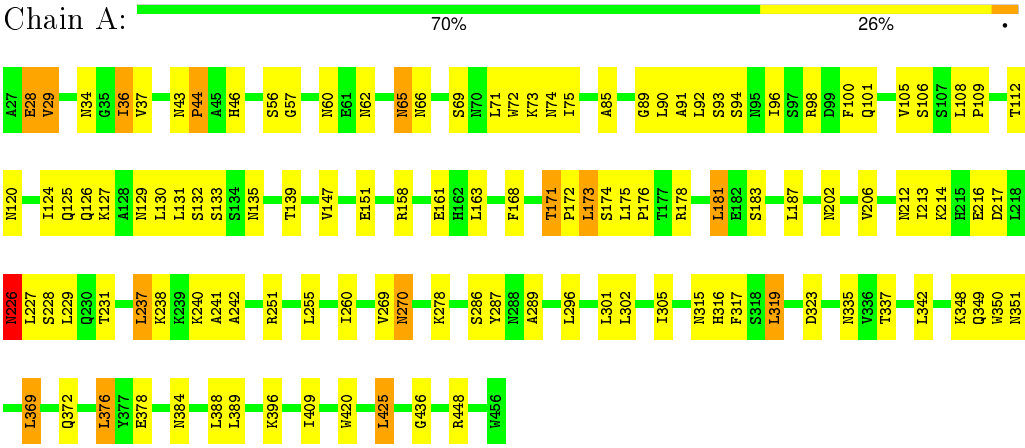
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

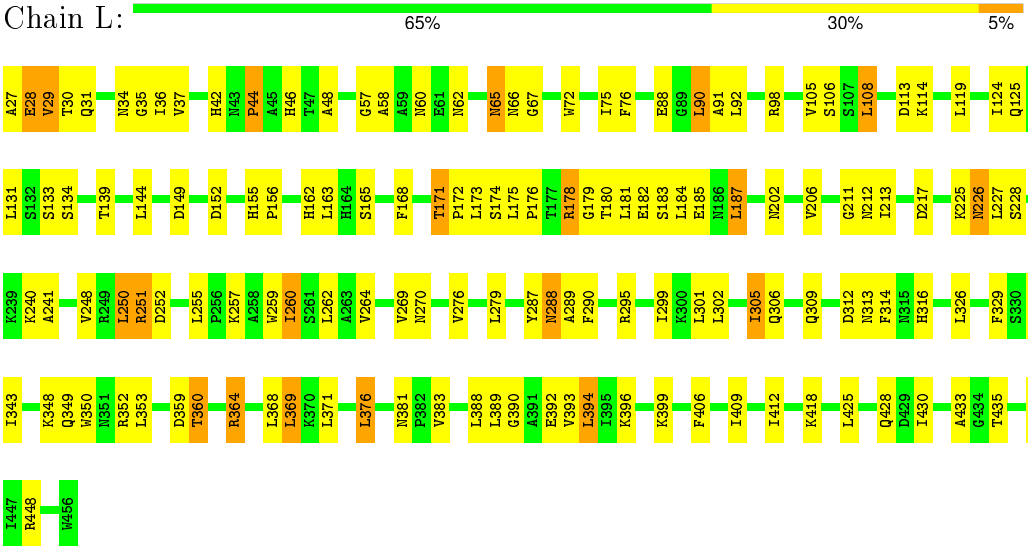
• Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

Chain A:



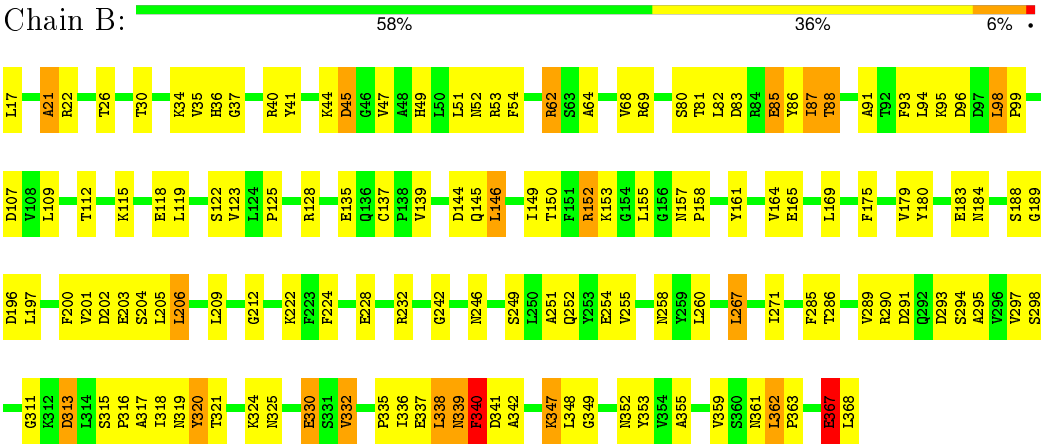
• Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

Chain L:



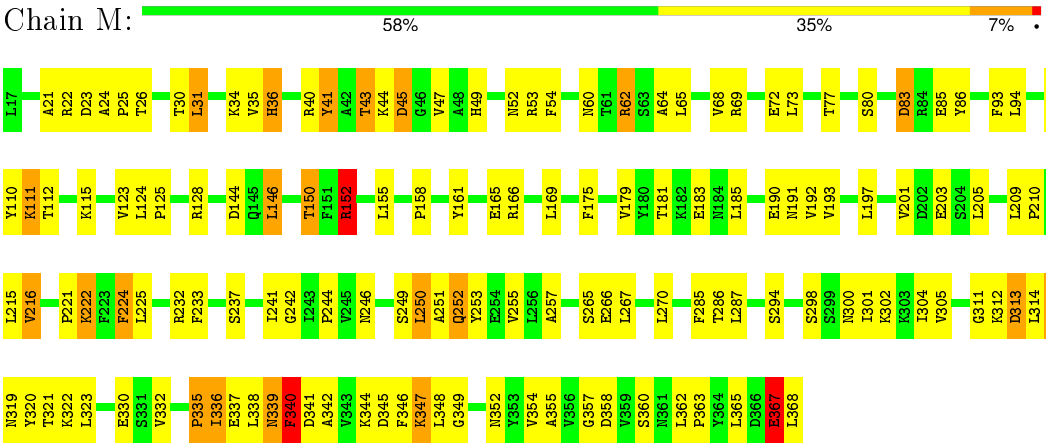
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



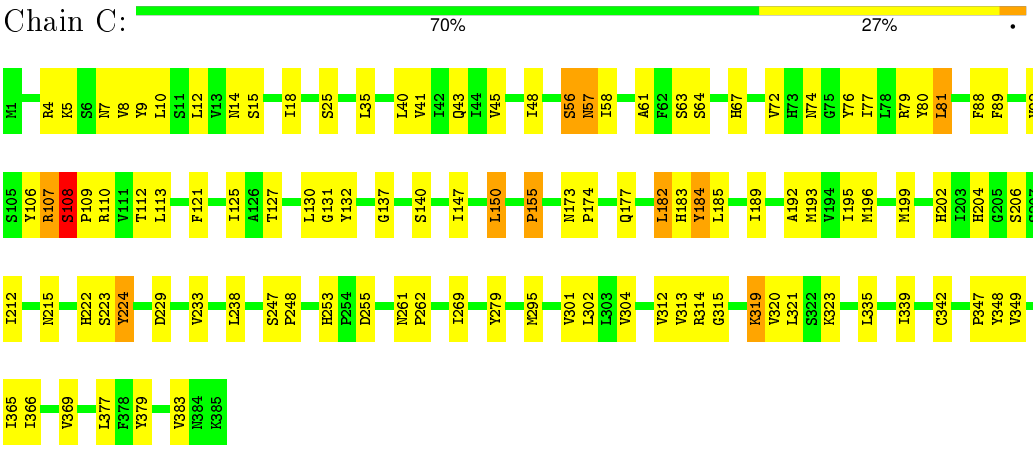
• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain M:



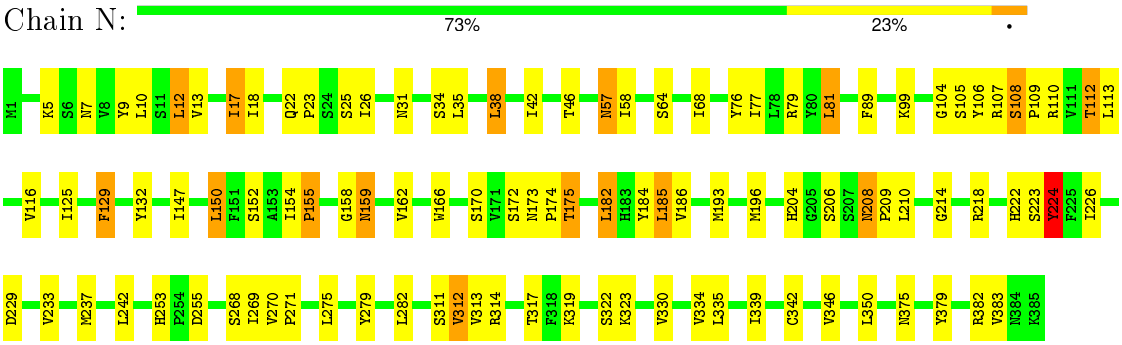
• Molecule 3: CYTOCHROME B

Chain C:



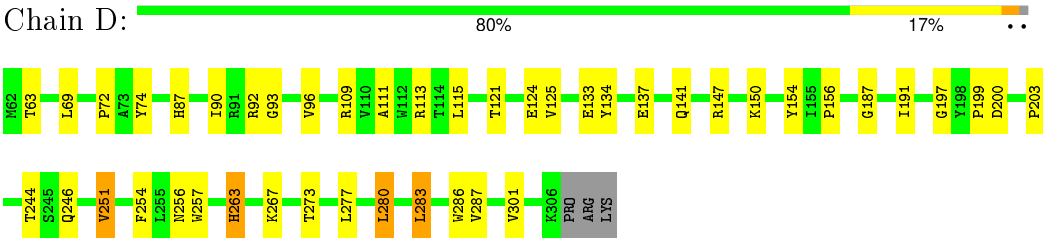
• Molecule 3: CYTOCHROME B

Chain N:



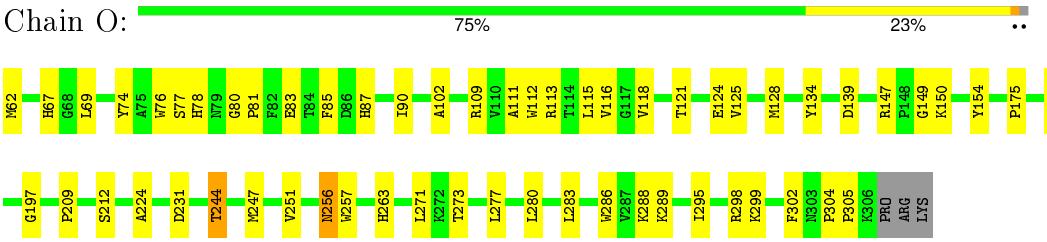
• Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain D:



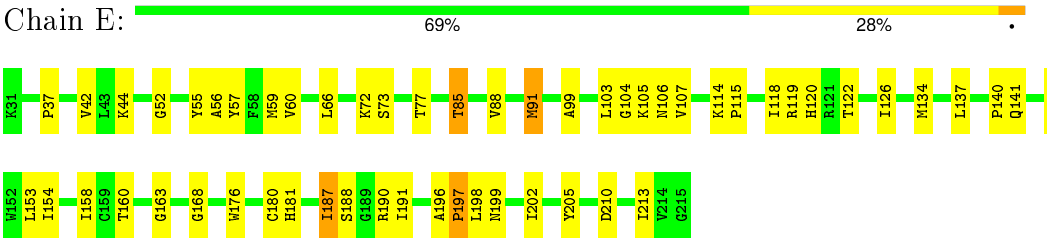
• Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain O:



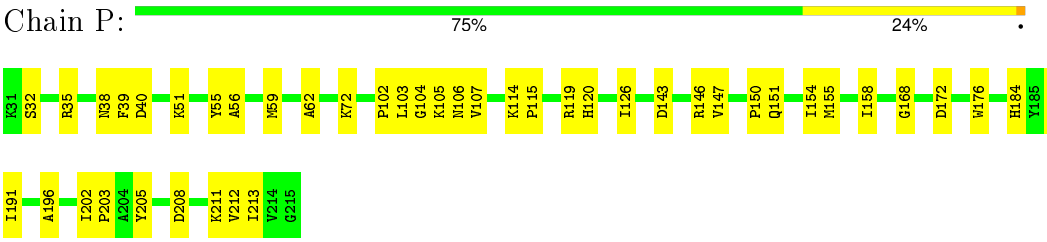
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E:



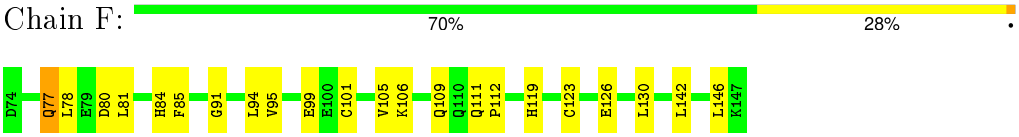
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain P:



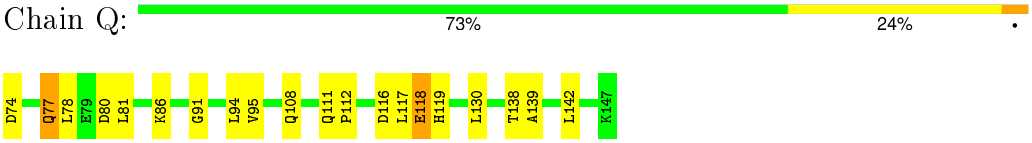
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN

Chain F:



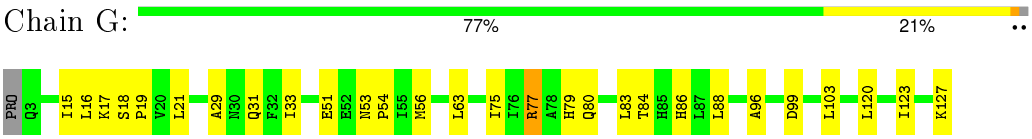
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN

Chain Q:



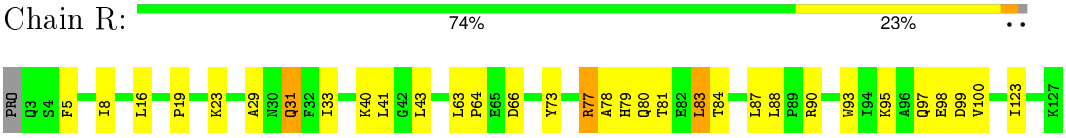
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain G:



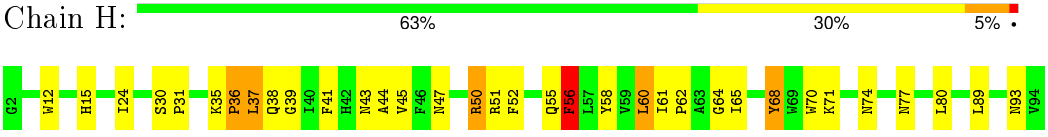
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain R:



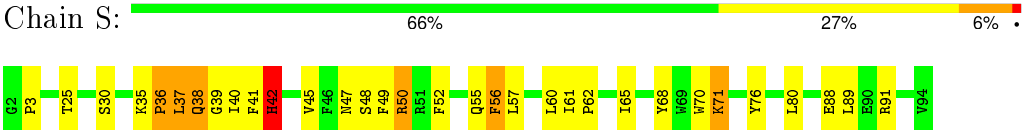
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain H:



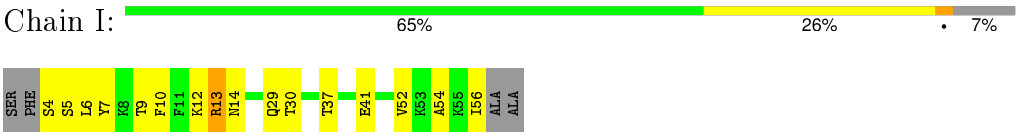
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain S:



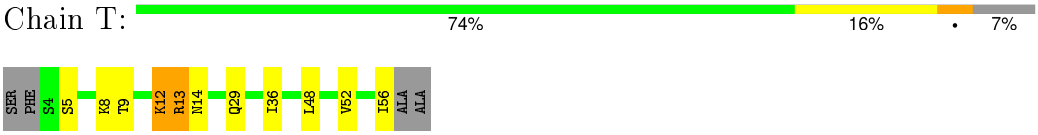
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I:



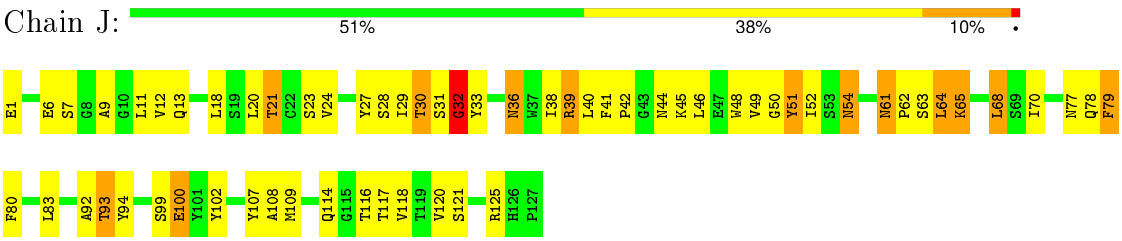
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain T:



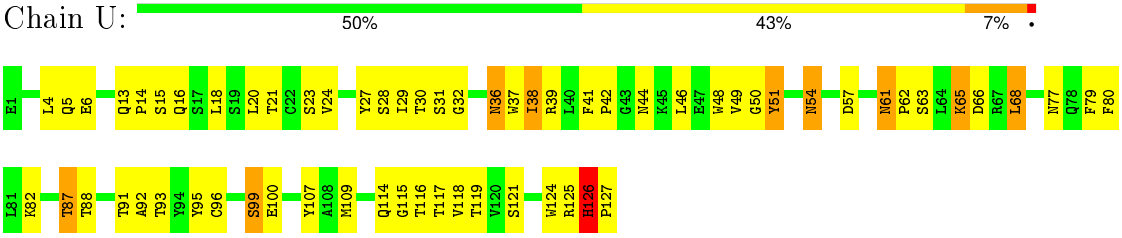
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain J:



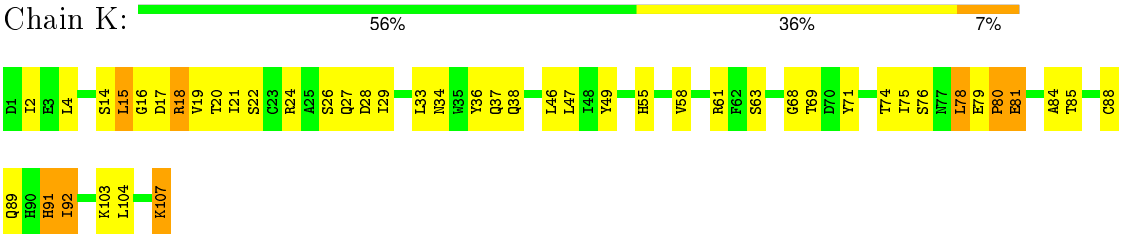
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain U:



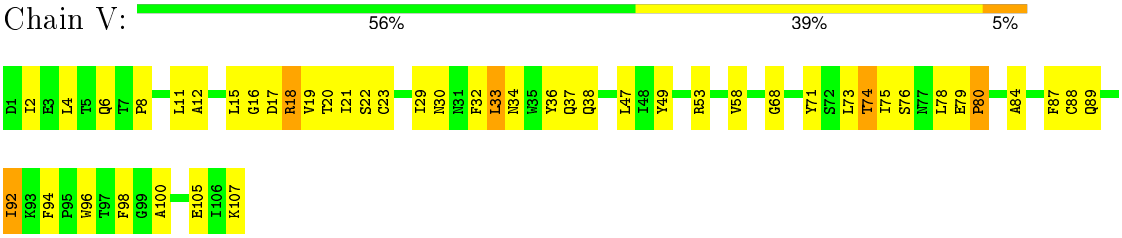
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K:



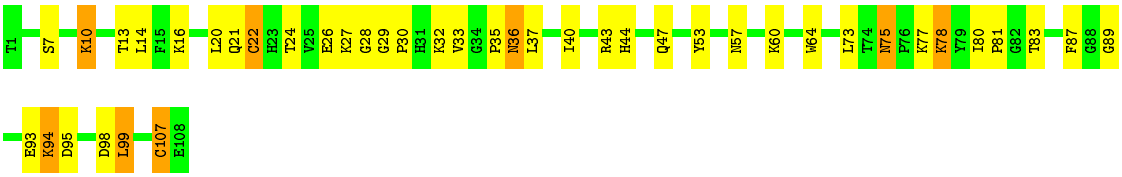
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain V:



• Molecule 12: CYTOCHROME C, ISO-1

Chain W:


T1
S7
K10
T13
L14
F15
K16
L20
Q21
C22
H23
T24
V25
E26
K27
G28
G29
P30
H31
K32
V33
G34
P35
N36
L37
I40
R43
H44
Q47
Y53
N57
K60
W64
L73
T74
N75
P76
K77
K78
Y79
I80
P81
G82
T83
F87
G88
G89
E93
K94
D95
D98
L99
C107
E108

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	147.22Å 165.53Å 195.89Å 90.00° 104.19° 90.00°	Depositor
Resolution (Å)	29.64 – 2.97	Depositor
% Data completeness (in resolution range)	93.7 (29.64-2.97)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35643	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, M3L, FES, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/3399	0.63	0/4606
1	L	0.40	0/3399	0.63	1/4606 (0.0%)
2	B	0.37	0/2781	0.68	2/3764 (0.1%)
2	M	0.38	0/2781	0.68	1/3764 (0.0%)
3	C	0.50	0/3191	0.68	0/4353
3	N	0.49	0/3191	0.70	0/4353
4	D	0.41	0/1989	0.64	0/2710
4	O	0.41	0/1989	0.63	0/2710
5	E	0.41	0/1444	0.67	1/1957 (0.1%)
5	P	0.39	0/1444	0.67	0/1957
6	F	0.39	0/639	0.59	0/859
6	Q	0.39	0/639	0.61	0/859
7	G	0.42	0/1032	0.69	0/1397
7	R	0.43	0/1032	0.68	0/1397
8	H	0.49	0/804	0.65	0/1088
8	S	0.52	0/804	0.61	0/1088
9	I	0.43	0/449	0.55	0/605
9	T	0.44	0/449	0.56	0/605
10	J	0.38	0/1043	0.68	1/1422 (0.1%)
10	U	0.38	0/1043	0.68	1/1422 (0.1%)
11	K	0.35	0/863	0.58	0/1172
11	V	0.36	0/863	0.62	0/1172
12	W	0.52	0/856	0.68	0/1145
All	All	0.42	0/36124	0.66	7/49011 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	32	GLY	N-CA-C	8.27	133.77	113.10
10	J	32	GLY	N-CA-C	6.98	130.55	113.10
2	B	340	PHE	N-CA-C	-6.37	93.80	111.00
2	M	340	PHE	N-CA-C	-6.34	93.87	111.00
5	E	163	GLY	N-CA-C	5.42	126.66	113.10
1	L	35	GLY	N-CA-C	-5.30	99.84	113.10
2	B	87	ILE	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	224	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3338	0	3316	87	0
1	L	3338	0	3316	101	0
2	B	2735	0	2774	98	0
2	M	2735	0	2774	107	0
3	C	3089	0	3125	87	0
3	N	3089	0	3125	84	0
4	D	1929	0	1844	25	0
4	O	1929	0	1844	43	0
5	E	1411	0	1386	49	0
5	P	1411	0	1386	38	0
6	F	625	0	576	11	0
6	Q	625	0	576	9	0
7	G	1012	0	1026	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	1012	0	1026	21	0
8	H	773	0	736	29	0
8	S	773	0	736	29	0
9	I	436	0	435	10	0
9	T	436	0	435	12	0
10	J	1015	0	959	48	0
10	U	1015	0	959	47	0
11	K	842	0	820	40	0
11	V	842	0	820	41	0
12	W	850	0	854	27	0
13	C	86	0	60	7	0
13	D	43	0	30	0	0
13	N	86	0	60	3	0
13	O	43	0	30	3	0
13	W	43	0	30	2	0
14	E	4	0	0	1	0
14	P	4	0	0	0	0
15	C	37	0	40	4	0
15	N	37	0	40	4	0
All	All	35643	0	35138	991	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (991) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:HIS:HD2	2:B:161:TYR:H	1.08	0.97
2:M:49:HIS:HD2	2:M:161:TYR:H	1.13	0.96
7:R:31:GLN:HE21	7:R:31:GLN:HA	1.31	0.96
1:L:62:ASN:H	1:L:65:ASN:HD21	1.13	0.95
1:A:62:ASN:HB2	1:A:65:ASN:HD21	1.31	0.95
3:N:58:ILE:H	3:N:173:ASN:ND2	1.64	0.95
1:L:62:ASN:H	1:L:65:ASN:ND2	1.65	0.94
3:N:7:ASN:HD22	3:N:10:LEU:H	0.99	0.93
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.32	0.93
2:B:98:LEU:HD11	2:B:192:VAL:HG13	1.49	0.92
2:B:83:ASP:HB2	2:B:86:TYR:H	1.35	0.92
6:F:77:GLN:NE2	6:F:77:GLN:H	1.67	0.91
2:M:98:LEU:HD11	2:M:192:VAL:HG13	1.53	0.91
2:B:347:LYS:HD3	2:B:347:LYS:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:77:GLN:HE21	6:F:77:GLN:H	0.97	0.89
2:B:49:HIS:CD2	2:B:161:TYR:H	1.89	0.89
10:U:29:ILE:H	10:U:77:ASN:HD21	1.21	0.88
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.40	0.87
1:A:62:ASN:HB2	1:A:65:ASN:ND2	1.91	0.85
1:L:57:GLY:H	1:L:60:ASN:HD22	1.24	0.85
2:M:49:HIS:CD2	2:M:161:TYR:H	1.96	0.84
6:F:77:GLN:HE21	6:F:77:GLN:N	1.75	0.84
2:M:300:ASN:O	2:M:304:ILE:HG12	1.78	0.83
5:P:172:ASP:H	5:P:184:HIS:HD2	1.24	0.82
1:L:237:LEU:HD23	1:L:237:LEU:H	1.43	0.82
5:E:187:ILE:H	5:E:187:ILE:HD12	1.45	0.81
2:M:110:TYR:HD2	2:M:205:LEU:HD23	1.46	0.81
5:P:72:LYS:NZ	9:T:29:GLN:HE22	1.77	0.81
10:U:54:ASN:H	10:U:54:ASN:HD22	1.27	0.81
3:N:7:ASN:ND2	3:N:10:LEU:H	1.79	0.80
8:H:35:LYS:HE2	8:H:36:PRO:HD2	1.64	0.80
1:A:120:ASN:HD21	1:A:124:ILE:HD12	1.46	0.80
10:J:61:ASN:HD22	10:J:63:SER:H	1.28	0.79
3:C:253:HIS:HD2	3:C:255:ASP:H	1.30	0.79
10:J:54:ASN:HD22	10:J:54:ASN:H	1.27	0.79
2:B:267:LEU:HD22	2:B:304:ILE:HD13	1.64	0.78
8:H:80:LEU:HB3	8:H:89:LEU:HD23	1.64	0.78
1:A:65:ASN:HA	1:A:187:LEU:HD11	1.65	0.77
8:H:41:PHE:HA	8:H:45:VAL:HB	1.65	0.77
3:N:159:ASN:H	3:N:159:ASN:HD22	1.33	0.77
1:L:57:GLY:H	1:L:60:ASN:ND2	1.81	0.77
10:U:6:GLU:H	10:U:114:GLN:HE21	1.33	0.77
4:O:62:MET:HB3	4:O:67:HIS:CE1	2.20	0.77
3:N:108:SER:CB	3:N:109:PRO:HD3	2.15	0.76
3:C:4:ARG:HE	3:C:14:ASN:ND2	1.84	0.76
5:E:191:ILE:HD13	5:E:196:ALA:HB3	1.67	0.76
3:C:125:ILE:HG22	15:C:505:SMA:H37	1.67	0.75
1:L:295:ARG:HD2	1:L:306:GLN:OE1	1.85	0.75
10:U:36:ASN:HD21	10:U:99:SER:HB3	1.52	0.75
4:D:197:GLY:O	4:D:199:PRO:HD3	1.86	0.75
2:M:60:ASN:HD22	2:M:111:LYS:HB2	1.52	0.75
3:N:13:VAL:HG13	3:N:17:ILE:HD12	1.67	0.75
11:V:36:TYR:CE2	11:V:89:GLN:HG2	2.21	0.74
1:L:316:HIS:HE1	1:L:350:TRP:HE1	1.36	0.74
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:172:ASP:H	5:P:184:HIS:CD2	2.05	0.74
4:O:111:ALA:HA	4:O:154:TYR:HA	1.68	0.73
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.69	0.73
1:L:260:ILE:HD11	1:L:343:ILE:HD11	1.71	0.73
2:B:318:ILE:HA	2:B:321:THR:HG22	1.70	0.73
3:C:56:SER:HB2	3:C:177:GLN:HG2	1.71	0.73
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.29	0.72
1:A:126:GLN:HG2	1:A:129:ASN:HB2	1.69	0.72
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.72	0.72
3:C:7:ASN:ND2	3:C:10:LEU:H	1.86	0.72
3:N:253:HIS:HD2	3:N:255:ASP:H	1.35	0.72
4:O:271:LEU:HD23	9:T:36:ILE:HG23	1.72	0.72
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.71	0.71
5:P:72:LYS:HZ2	9:T:29:GLN:HE22	1.36	0.71
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.05	0.71
10:U:100:GLU:O	10:U:107:TYR:HA	1.91	0.71
10:U:41:PHE:HD2	10:U:92:ALA:HB2	1.56	0.71
5:E:72:LYS:NZ	9:I:29:GLN:HE21	1.89	0.71
1:A:72:TRP:CE3	1:A:75:ILE:HD11	2.26	0.71
1:A:316:HIS:HE1	1:A:350:TRP:HE1	1.38	0.71
4:O:289:LYS:NZ	8:S:40:ILE:HD11	2.06	0.71
11:V:34:ASN:HD22	11:V:49:TYR:HA	1.55	0.70
3:N:7:ASN:ND2	3:N:9:TYR:H	1.89	0.70
1:A:62:ASN:CB	1:A:65:ASN:HD21	2.04	0.70
5:E:44:LYS:NZ	5:E:52:GLY:H	1.89	0.70
5:P:103:LEU:HA	5:P:120:HIS:ND1	2.07	0.70
3:C:335:LEU:O	3:C:339:ILE:HG12	1.92	0.70
6:Q:77:GLN:HE21	6:Q:77:GLN:H	1.40	0.70
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.72	0.70
3:N:208:ASN:HD22	3:N:210:LEU:H	1.40	0.70
3:N:107:ARG:HD3	3:N:314:ARG:HG3	1.73	0.70
2:M:347:LYS:HG2	2:M:348:LEU:H	1.57	0.69
10:J:99:SER:HB3	10:J:109:MET:HG2	1.74	0.69
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.57	0.69
1:A:369:LEU:HD13	1:A:409:ILE:HD13	1.75	0.69
2:B:197:LEU:O	2:B:201:VAL:HG23	1.93	0.69
2:M:183:GLU:HB2	2:M:212:GLY:O	1.94	0.68
2:M:62:ARG:HB2	2:M:62:ARG:HH21	1.58	0.68
10:U:61:ASN:HD22	10:U:63:SER:H	1.41	0.68
3:C:108:SER:OG	3:C:109:PRO:HD2	1.93	0.68
11:K:2:ILE:HD12	11:K:2:ILE:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:108:SER:HB3	3:N:109:PRO:HD3	1.75	0.67
2:B:318:ILE:HD13	2:B:341:ASP:H	1.58	0.67
4:O:147:ARG:HH21	4:O:150:LYS:HE3	1.57	0.67
2:B:34:LYS:HG3	2:B:88:THR:HG23	1.76	0.67
10:J:107:TYR:H	11:K:91:HIS:CD2	2.12	0.67
3:C:301:VAL:O	3:C:304:VAL:HG12	1.93	0.67
5:E:134:MET:HG2	10:J:31:SER:HB3	1.77	0.67
4:O:125:VAL:HA	4:O:128:MET:HE3	1.77	0.67
8:S:38:GLN:O	8:S:40:ILE:HD12	1.95	0.67
2:B:337:GLU:O	2:B:339:ASN:N	2.28	0.67
7:G:123:ILE:O	1:L:360:THR:HG21	1.95	0.66
2:B:340:PHE:O	2:B:341:ASP:HB2	1.95	0.66
2:M:40:ARG:HD3	2:M:155:LEU:HG	1.77	0.66
10:J:41:PHE:HD1	10:J:45:LYS:HG3	1.60	0.66
10:U:54:ASN:HD22	10:U:54:ASN:N	1.94	0.66
3:N:108:SER:OG	3:N:109:PRO:HD3	1.96	0.66
3:C:173:ASN:HB3	3:C:174:PRO:HD3	1.78	0.66
7:R:31:GLN:NE2	7:R:31:GLN:HA	2.07	0.66
1:L:376:LEU:HD22	1:L:388:LEU:HD11	1.78	0.66
2:B:62:ARG:CB	2:B:62:ARG:HH21	2.09	0.66
1:A:348:LYS:HD3	1:A:351:ASN:OD1	1.95	0.66
3:C:279:TYR:CE1	15:C:505:SMA:H5	2.30	0.65
3:N:17:ILE:HG22	3:N:226:ILE:HD11	1.78	0.65
12:W:33:VAL:O	13:W:526:HEM:HMD3	1.96	0.65
3:C:253:HIS:CD2	3:C:255:ASP:H	2.14	0.65
1:L:108:LEU:HD22	2:M:323:LEU:HD23	1.78	0.65
3:N:58:ILE:H	3:N:173:ASN:HD22	1.45	0.65
3:C:7:ASN:HD22	3:C:10:LEU:H	1.43	0.65
3:N:7:ASN:HD22	3:N:10:LEU:N	1.83	0.65
11:V:2:ILE:H	11:V:2:ILE:HD12	1.62	0.65
6:Q:77:GLN:NE2	6:Q:77:GLN:H	1.93	0.65
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.78	0.64
2:M:69:ARG:O	2:M:73:LEU:HD23	1.97	0.64
3:N:104:GLY:HA2	3:N:106:TYR:CE2	2.31	0.64
10:U:29:ILE:H	10:U:77:ASN:ND2	1.93	0.64
3:C:58:ILE:H	3:C:173:ASN:ND2	1.95	0.64
11:V:32:PHE:HB2	11:V:92:ILE:HG22	1.78	0.64
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.79	0.64
1:A:147:VAL:HG22	1:A:178:ARG:HB3	1.79	0.64
3:N:147:ILE:O	3:N:150:LEU:HB2	1.98	0.64
10:J:29:ILE:H	10:J:77:ASN:HD21	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:311:SER:CB	3:N:319:LYS:HZ1	2.10	0.64
11:V:74:THR:HG22	11:V:75:ILE:H	1.63	0.64
2:B:44:LYS:O	2:B:47:VAL:HG23	1.98	0.63
10:U:29:ILE:HG12	10:U:77:ASN:ND2	2.13	0.63
2:M:347:LYS:HD3	2:M:347:LYS:H	1.62	0.63
3:N:25:SER:OG	7:R:79:HIS:HD2	1.82	0.63
1:L:228:SER:HB3	1:L:231:THR:HB	1.81	0.63
2:M:365:LEU:HD12	2:M:368:LEU:HD12	1.80	0.63
3:N:147:ILE:HA	3:N:150:LEU:HD22	1.80	0.63
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.81	0.63
5:P:32:SER:HB3	5:P:35:ARG:HG3	1.81	0.63
3:C:108:SER:CB	3:C:109:PRO:HD2	2.28	0.63
3:N:379:TYR:CE1	3:N:383:VAL:HG21	2.33	0.62
1:A:296:LEU:O	2:B:69:ARG:NH2	2.31	0.62
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.81	0.62
2:B:49:HIS:HD2	2:B:161:TYR:N	1.91	0.62
2:M:347:LYS:HG2	2:M:348:LEU:N	2.13	0.62
1:A:66:ASN:ND2	1:A:175:LEU:HD12	2.13	0.62
2:M:355:ALA:HB1	2:M:362:LEU:HD23	1.82	0.62
7:R:80:GLN:O	7:R:84:THR:HG23	1.98	0.62
2:M:337:GLU:O	2:M:339:ASN:N	2.33	0.62
2:M:340:PHE:O	2:M:341:ASP:HB2	2.00	0.62
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.35	0.62
1:L:67:GLY:HA3	1:L:184:LEU:CD1	2.29	0.61
1:L:67:GLY:HA3	1:L:184:LEU:HD11	1.82	0.61
5:E:181:HIS:HB2	14:E:504:FES:S1	2.40	0.61
9:T:12:LYS:O	9:T:13:ARG:HG3	2.01	0.61
3:C:208:ASN:HD22	3:C:210:LEU:H	1.46	0.61
7:R:87:LEU:HG	8:S:50:ARG:HH11	1.65	0.61
1:L:62:ASN:N	1:L:65:ASN:HD21	1.92	0.61
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.81	0.61
10:U:28:SER:HB3	10:U:30:THR:HG22	1.82	0.61
5:P:106:ASN:ND2	5:P:119:ARG:HH21	1.99	0.61
11:V:38:GLN:O	11:V:84:ALA:HB1	2.01	0.61
11:K:36:TYR:CE2	11:K:89:GLN:HG2	2.30	0.61
2:M:340:PHE:C	2:M:342:ALA:H	2.02	0.61
10:U:93:THR:HG22	10:U:117:THR:HG23	1.82	0.61
1:L:288:ASN:C	1:L:288:ASN:HD22	2.03	0.60
12:W:13:THR:HA	12:W:16:LYS:HE2	1.83	0.60
2:B:164:VAL:HG21	2:M:232:ARG:NH1	2.16	0.60
3:C:132:TYR:HA	13:C:501:HEM:HAA2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:HIS:CE1	1:A:350:TRP:HE1	2.19	0.60
12:W:29:GLY:HA2	12:W:36:ASN:OD1	2.01	0.60
2:M:257:ALA:HB2	2:M:285:PHE:HE1	1.66	0.60
1:L:288:ASN:ND2	1:L:290:PHE:H	2.00	0.60
5:E:107:VAL:CG1	5:E:118:ILE:HB	2.31	0.60
2:M:44:LYS:O	2:M:47:VAL:HG23	2.02	0.60
11:K:17:ASP:HB2	11:K:18:ARG:HH22	1.66	0.60
11:V:75:ILE:HG22	11:V:76:SER:N	2.16	0.60
3:N:275:LEU:HD13	15:N:525:SMA:H14	1.83	0.60
3:N:58:ILE:H	3:N:173:ASN:HD21	1.49	0.60
8:S:40:ILE:HD12	8:S:40:ILE:H	1.66	0.60
3:N:64:SER:O	3:N:68:ILE:HG13	2.02	0.60
2:B:45:ASP:HB2	2:B:165:GLU:HG2	1.84	0.60
3:N:166:TRP:HA	3:N:175:THR:HG23	1.84	0.60
12:W:13:THR:HG22	12:W:16:LYS:HE2	1.83	0.59
10:U:91:THR:HG23	10:U:119:THR:HA	1.84	0.59
6:F:91:GLY:O	6:F:95:VAL:HG13	2.01	0.59
1:L:264:VAL:HG12	1:L:430:ILE:HG22	1.83	0.59
2:M:312:LYS:O	2:M:313:ASP:HB2	2.02	0.59
3:C:347:PRO:HG3	8:H:77:ASN:HB2	1.84	0.59
4:O:147:ARG:NH2	4:O:150:LYS:HE3	2.16	0.59
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.84	0.59
2:B:152:ARG:HG3	2:B:152:ARG:HH21	1.67	0.59
1:L:287:TYR:HB3	1:L:314:PHE:CE2	2.38	0.59
1:L:227:LEU:HG	1:L:228:SER:H	1.67	0.59
8:H:61:ILE:O	8:H:65:ILE:HG13	2.03	0.59
13:C:501:HEM:HHD	13:C:501:HEM:HBC2	1.85	0.59
10:U:16:GLN:HE21	10:U:16:GLN:HA	1.68	0.59
10:J:49:VAL:HG13	10:J:64:LEU:HD12	1.85	0.59
11:K:17:ASP:O	11:K:78:LEU:HD13	2.03	0.58
1:A:227:LEU:HG	1:A:228:SER:H	1.68	0.58
1:A:168:PHE:O	1:A:174:SER:HB3	2.03	0.58
1:A:214:LYS:HB2	1:A:217:ASP:HB2	1.84	0.58
11:V:17:ASP:HB2	11:V:18:ARG:NH2	2.18	0.58
1:A:75:ILE:HG23	1:A:139:THR:HG21	1.85	0.58
8:S:80:LEU:HB3	8:S:89:LEU:HD23	1.84	0.58
5:E:187:ILE:N	5:E:187:ILE:HD12	2.17	0.58
11:K:55:HIS:O	11:K:58:VAL:HG22	2.04	0.58
2:M:62:ARG:CB	2:M:62:ARG:HH21	2.15	0.58
5:P:102:PRO:HB2	5:P:105:LYS:HG2	1.85	0.58
5:E:99:ALA:HB2	5:E:210:ASP:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:208:ASN:HD22	3:N:210:LEU:N	2.00	0.58
1:L:171:THR:HG23	1:L:172:PRO:HD2	1.85	0.58
1:A:171:THR:HG23	1:A:172:PRO:HD2	1.85	0.58
11:K:63:SER:HB2	11:K:74:THR:HB	1.85	0.58
2:M:155:LEU:HD12	2:M:155:LEU:N	2.19	0.58
12:W:57:ASN:HD21	13:W:526:HEM:HAA2	1.67	0.58
10:J:61:ASN:ND2	10:J:63:SER:H	1.99	0.58
8:H:52:PHE:O	8:H:56:PHE:HB3	2.03	0.58
4:O:286:TRP:CE3	5:P:59:MET:HG3	2.38	0.58
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.44	0.58
1:A:237:LEU:H	1:A:237:LEU:HD23	1.68	0.58
10:U:29:ILE:N	10:U:77:ASN:HD21	1.98	0.57
3:C:7:ASN:HD22	3:C:10:LEU:N	2.02	0.57
1:L:250:LEU:HD23	8:S:25:THR:HG23	1.86	0.57
2:B:105:LEU:O	2:B:109:LEU:HD12	2.04	0.57
1:L:36:ILE:HG12	1:L:202:ASN:OD1	2.05	0.57
1:L:316:HIS:CE1	1:L:350:TRP:HE1	2.20	0.57
12:W:35:PRO:HG3	12:W:53:TYR:CE1	2.40	0.57
2:B:146:LEU:HD23	2:B:286:THR:HG22	1.86	0.57
2:M:252:GLN:O	2:M:255:VAL:HG22	2.03	0.57
12:W:27:LYS:HD2	12:W:28:GLY:N	2.20	0.57
1:A:65:ASN:N	1:A:65:ASN:HD22	2.01	0.57
7:R:29:ALA:O	7:R:33:ILE:HG13	2.05	0.57
1:A:216:GLU:HA	1:A:219:VAL:HG12	1.86	0.57
1:A:37:VAL:HG13	1:A:206:VAL:HG22	1.87	0.57
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.85	0.57
1:A:183:SER:O	1:A:187:LEU:HD13	2.05	0.57
4:O:121:THR:OG1	4:O:124:GLU:HG3	2.05	0.57
5:P:154:ILE:HB	5:P:205:TYR:CE1	2.40	0.57
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.20	0.57
12:W:27:LYS:HD2	12:W:28:GLY:H	1.69	0.57
8:S:41:PHE:H	8:S:45:VAL:HB	1.69	0.57
3:C:4:ARG:NE	3:C:14:ASN:ND2	2.53	0.56
3:C:109:PRO:HB2	3:C:204:HIS:CE1	2.40	0.56
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.87	0.56
5:E:197:PRO:O	5:E:198:LEU:HD23	2.05	0.56
1:L:91:ALA:HB3	1:L:106:SER:HB2	1.86	0.56
7:R:43:LEU:HD21	7:R:78:ALA:HB2	1.87	0.56
1:L:390:GLY:O	1:L:394:LEU:HB2	2.05	0.56
2:B:367:GLU:O	2:B:368:LEU:HB2	2.04	0.56
10:J:38:ILE:HD12	10:J:46:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:335:LEU:O	3:N:339:ILE:HG12	2.05	0.56
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.87	0.56
1:L:48:ALA:HA	1:L:211:GLY:HA3	1.87	0.56
2:M:347:LYS:HD3	2:M:347:LYS:N	2.20	0.56
10:J:39:ARG:NH2	10:J:41:PHE:HZ	2.03	0.56
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.87	0.56
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.87	0.56
4:O:118:VAL:HG11	4:O:257:TRP:CE2	2.40	0.56
12:W:24:THR:HG23	12:W:32:LYS:HE2	1.88	0.56
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.86	0.56
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.86	0.56
10:J:62:PRO:O	10:J:65:LYS:HG2	2.06	0.56
3:N:132:TYR:HA	13:N:521:HEM:HAA2	1.87	0.56
5:E:147:VAL:HG21	5:E:150:PRO:HA	1.87	0.56
1:L:381:ASN:OD1	1:L:383:VAL:HG22	2.05	0.56
6:Q:91:GLY:O	6:Q:95:VAL:HG13	2.06	0.56
7:G:80:GLN:O	7:G:84:THR:HG23	2.06	0.56
1:L:37:VAL:HG13	1:L:206:VAL:HG22	1.87	0.56
10:J:6:GLU:H	10:J:114:GLN:HE21	1.52	0.56
1:A:72:TRP:CH2	1:A:131:LEU:HD21	2.41	0.55
1:A:301:LEU:HB2	1:A:349:GLN:HG3	1.88	0.55
1:L:29:VAL:HG11	1:L:399:LYS:HB3	1.87	0.55
5:E:72:LYS:HZ2	9:I:29:GLN:HE21	1.53	0.55
5:P:187:ILE:H	5:P:187:ILE:HD12	1.71	0.55
5:P:72:LYS:HZ1	9:T:29:GLN:HE22	1.54	0.55
11:K:74:THR:HG22	11:K:75:ILE:N	2.21	0.55
3:C:58:ILE:H	3:C:173:ASN:HD22	1.52	0.55
1:A:36:ILE:HG22	1:A:37:VAL:H	1.70	0.55
1:L:75:ILE:HG22	1:L:139:THR:HG21	1.89	0.55
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.40	0.55
4:O:295:ILE:O	4:O:298:ARG:HB2	2.05	0.55
1:L:183:SER:O	1:L:187:LEU:HD13	2.07	0.55
3:C:77:ILE:O	3:C:81:LEU:HB2	2.06	0.55
5:E:190:ARG:HA	5:E:199:ASN:HB3	1.88	0.55
2:M:335:PRO:HG2	2:M:336:ILE:HG13	1.88	0.55
10:J:36:ASN:H	10:J:36:ASN:HD22	1.55	0.55
1:L:75:ILE:HG13	1:L:76:PHE:N	2.21	0.55
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.41	0.55
2:B:150:THR:HG22	2:B:352:ASN:HD22	1.69	0.54
8:S:48:SER:C	8:S:50:ARG:H	2.10	0.54
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:SER:O	3:C:202:HIS:HE1	1.90	0.54
5:P:155:MET:HA	5:P:203:PRO:HD2	1.88	0.54
6:Q:111:GLN:HB3	6:Q:112:PRO:HD2	1.89	0.54
5:E:122:THR:O	5:E:126:ILE:HG13	2.07	0.54
11:V:75:ILE:HG22	11:V:76:SER:H	1.71	0.54
1:A:287:TYR:CD2	1:A:302:LEU:HD21	2.43	0.54
2:B:271:ILE:HG22	2:B:289:VAL:HG22	1.89	0.54
10:U:13:GLN:HA	10:U:121:SER:O	2.07	0.54
2:B:40:ARG:HH11	2:B:85:GLU:HG3	1.73	0.54
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.07	0.54
2:B:146:LEU:O	2:B:150:THR:HG23	2.07	0.54
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.22	0.54
2:B:202:ASP:O	2:B:203:GLU:HG2	2.08	0.54
3:C:108:SER:OG	3:C:314:ARG:NH2	2.41	0.54
3:C:253:HIS:HD2	3:C:255:ASP:N	2.01	0.54
1:A:98:ARG:HD3	1:A:173:LEU:HD12	1.89	0.54
1:A:228:SER:HB3	1:A:231:THR:HB	1.90	0.54
8:S:76:TYR:O	8:S:80:LEU:HG	2.08	0.54
1:L:162:HIS:HA	1:L:165:SER:HB3	1.90	0.54
1:L:42:HIS:HB3	1:L:213:ILE:O	2.08	0.54
10:U:6:GLU:N	10:U:114:GLN:HE21	2.05	0.53
10:J:18:LEU:HD11	10:J:118:VAL:HG11	1.89	0.53
5:E:56:ALA:O	5:E:60:VAL:HG23	2.07	0.53
11:K:107:LYS:HA	11:K:107:LYS:HE3	1.89	0.53
1:A:147:VAL:HG12	1:A:181:LEU:HD23	1.90	0.53
1:L:72:TRP:CZ3	1:L:75:ILE:HD11	2.43	0.53
2:B:36:HIS:HB3	2:B:41:TYR:CE1	2.43	0.53
1:A:57:GLY:H	1:A:60:ASN:HD22	1.56	0.53
10:J:28:SER:HB2	10:J:31:SER:OG	2.08	0.53
2:B:246:ASN:HD22	2:B:249:SER:HB2	1.73	0.53
3:N:223:SER:O	3:N:224:TYR:CG	2.62	0.53
11:K:27:GLN:HG2	11:K:28:ASP:H	1.73	0.53
3:N:108:SER:CB	3:N:109:PRO:CD	2.86	0.53
2:M:246:ASN:HD22	2:M:249:SER:HB3	1.73	0.53
2:B:313:ASP:C	2:B:315:SER:H	2.12	0.53
1:A:37:VAL:CG1	1:A:206:VAL:HG22	2.39	0.53
3:N:323:LYS:HE3	8:S:55:GLN:HE22	1.73	0.53
2:M:52:ASN:ND2	2:M:80:SER:OG	2.41	0.53
2:M:237:SER:HA	2:M:357:GLY:HA3	1.90	0.53
2:B:51:LEU:HD11	2:B:180:TYR:HE1	1.74	0.53
1:L:44:PRO:HA	1:L:212:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:109:PRO:HB2	3:N:204:HIS:CE1	2.44	0.53
3:C:76:TYR:CE1	3:C:77:ILE:HG13	2.43	0.53
11:V:47:LEU:HA	11:V:58:VAL:HG11	1.90	0.53
1:L:31:GLN:HE22	1:L:393:VAL:HB	1.74	0.53
10:J:33:TYR:CD2	10:J:33:TYR:N	2.77	0.53
2:M:205:LEU:HD12	2:M:205:LEU:N	2.23	0.52
3:C:193:MET:HA	3:C:193:MET:CE	2.39	0.52
5:P:186:ASP:OD2	5:P:190:ARG:NH2	2.42	0.52
7:G:120:LEU:HD13	2:M:69:ARG:HG3	1.90	0.52
3:N:268:SER:O	3:N:270:VAL:HG23	2.09	0.52
2:M:146:LEU:HD23	2:M:286:THR:HG22	1.92	0.52
12:W:7:SER:OG	12:W:10:LYS:HB2	2.10	0.52
1:A:65:ASN:H	1:A:65:ASN:HD22	1.56	0.52
8:S:35:LYS:O	8:S:37:LEU:N	2.42	0.52
10:U:61:ASN:ND2	10:U:63:SER:H	2.07	0.52
2:M:250:LEU:HD23	2:M:251:ALA:H	1.75	0.52
7:G:63:LEU:HD13	7:G:103:LEU:CD1	2.40	0.52
4:O:289:LYS:HZ3	8:S:40:ILE:HD11	1.73	0.52
5:E:57:TYR:HB3	9:I:7:TYR:OH	2.09	0.52
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.53	0.52
2:B:339:ASN:HA	2:B:342:ALA:HB3	1.90	0.52
3:N:77:ILE:O	3:N:81:LEU:HB2	2.09	0.52
2:M:41:TYR:O	2:M:175:PHE:HE1	1.93	0.52
1:L:178:ARG:HH21	1:L:178:ARG:HG2	1.75	0.52
10:U:54:ASN:H	10:U:54:ASN:ND2	2.03	0.52
1:A:75:ILE:CG2	1:A:139:THR:HG21	2.40	0.52
8:H:12:TRP:NE1	8:S:3:PRO:HB3	2.25	0.52
4:O:224:ALA:HB3	13:O:523:HEM:HBD2	1.92	0.52
1:A:66:ASN:HD21	1:A:176:PRO:HD2	1.75	0.52
3:C:193:MET:HE2	3:C:196:MET:SD	2.49	0.52
2:M:34:LYS:HB3	2:M:86:TYR:CD1	2.45	0.52
11:V:17:ASP:O	11:V:78:LEU:HD13	2.10	0.52
1:L:178:ARG:HD2	1:L:178:ARG:H	1.74	0.52
1:L:349:GLN:HE22	1:L:352:ARG:HH21	1.57	0.52
2:B:317:ALA:O	2:B:320:TYR:HB3	2.10	0.52
1:A:151:GLU:HA	1:A:158:ARG:HD2	1.92	0.52
7:R:98:GLU:O	7:R:100:VAL:HG23	2.09	0.52
3:N:105:SER:CB	13:N:522:HEM:HBD2	2.40	0.52
3:N:110:ARG:O	3:N:113:LEU:HB3	2.10	0.51
11:K:103:LYS:HG3	11:K:104:LEU:N	2.25	0.51
11:V:15:LEU:HD12	11:V:15:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:289:LYS:HZ2	8:S:40:ILE:HD11	1.72	0.51
11:K:74:THR:HG22	11:K:75:ILE:H	1.74	0.51
8:H:50:ARG:HE	8:H:51:ARG:HH21	1.58	0.51
2:M:315:SER:HB3	2:M:344:LYS:HB2	1.91	0.51
3:N:105:SER:HB3	13:N:522:HEM:HBD2	1.91	0.51
2:M:318:ILE:O	2:M:319:ASN:HB2	2.09	0.51
10:J:40:LEU:HB3	10:J:93:THR:HG23	1.90	0.51
1:L:163:LEU:HD12	1:L:326:LEU:HD13	1.93	0.51
10:U:4:LEU:HG	10:U:24:VAL:HG22	1.93	0.51
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.91	0.51
7:G:18:SER:HB3	7:G:21:LEU:HD23	1.93	0.51
3:N:193:MET:HE2	3:N:193:MET:HA	1.93	0.51
10:J:36:ASN:N	10:J:36:ASN:ND2	2.59	0.51
1:L:252:ASP:HB3	1:L:255:LEU:HD12	1.91	0.51
2:M:35:VAL:HG12	2:M:179:VAL:HG12	1.91	0.51
3:N:253:HIS:CD2	3:N:255:ASP:HB2	2.45	0.51
3:C:104:GLY:O	3:C:107:ARG:HG3	2.11	0.51
11:K:15:LEU:HD12	11:K:15:LEU:N	2.25	0.51
3:C:189:ILE:O	3:C:192:ALA:HB3	2.11	0.51
2:B:205:LEU:HD12	2:B:205:LEU:H	1.76	0.51
4:O:289:LYS:HB2	8:S:37:LEU:HD13	1.93	0.51
10:U:28:SER:HB2	10:U:31:SER:OG	2.11	0.51
3:N:152:SER:HB3	3:N:162:VAL:HG21	1.92	0.51
2:M:225:LEU:HD21	2:M:244:PRO:HD2	1.93	0.51
5:P:172:ASP:N	5:P:184:HIS:HD2	2.03	0.51
2:M:155:LEU:HD12	2:M:155:LEU:H	1.76	0.51
3:C:193:MET:HA	3:C:193:MET:HE2	1.92	0.51
7:R:19:PRO:O	7:R:23:LYS:HG3	2.11	0.51
1:L:250:LEU:O	1:L:435:THR:HA	2.10	0.51
1:L:444:TYR:CE2	8:S:30:SER:HB2	2.46	0.51
6:Q:117:LEU:O	6:Q:118:GLU:HG3	2.10	0.51
3:C:195:ILE:O	3:C:199:MET:HG3	2.11	0.51
2:B:139:VAL:HG13	2:B:290:ARG:HD2	1.93	0.50
1:A:36:ILE:HG23	1:A:202:ASN:OD1	2.12	0.50
1:L:301:LEU:HB2	1:L:349:GLN:HG3	1.92	0.50
5:P:51:LYS:HE2	5:P:55:TYR:HE2	1.75	0.50
3:N:125:ILE:CG2	15:N:525:SMA:H37	2.42	0.50
4:O:273:THR:HG22	4:O:277:LEU:HD12	1.92	0.50
1:A:255:LEU:HD12	1:A:436:GLY:HA2	1.93	0.50
9:I:5:SER:O	9:I:9:THR:HG23	2.12	0.50
3:N:125:ILE:HG22	15:N:525:SMA:H37	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:72:LYS:HZ3	9:I:29:GLN:HE21	1.58	0.50
2:M:146:LEU:HD13	2:M:354:VAL:CG2	2.42	0.50
2:B:52:ASN:HD21	2:B:80:SER:C	2.15	0.50
4:O:134:TYR:CE2	4:O:149:GLY:HA3	2.47	0.50
11:V:12:ALA:HB1	11:V:105:GLU:O	2.11	0.50
11:V:11:LEU:HG	11:V:12:ALA:H	1.77	0.50
11:K:19:VAL:HG22	11:K:20:THR:N	2.27	0.50
2:B:300:ASN:O	2:B:304:ILE:HG12	2.12	0.50
11:V:29:ILE:HD11	11:V:71:TYR:CE1	2.47	0.50
8:S:41:PHE:O	8:S:42:HIS:HB2	2.10	0.50
2:M:65:LEU:O	2:M:69:ARG:HG2	2.12	0.50
3:N:182:LEU:O	3:N:186:VAL:HG23	2.12	0.50
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.00	0.50
2:B:103:ASN:O	2:B:107:ASP:HB2	2.12	0.50
7:R:40:LYS:HD3	7:R:93:TRP:CH2	2.47	0.50
1:A:65:ASN:H	1:A:65:ASN:ND2	2.09	0.49
3:C:315:GLY:O	3:C:319:LYS:HD2	2.11	0.49
2:B:255:VAL:HA	2:B:321:THR:OG1	2.12	0.49
4:D:280:LEU:HD11	5:E:66:LEU:HB2	1.92	0.49
2:M:98:LEU:N	2:M:99:PRO:HD2	2.27	0.49
2:B:62:ARG:HB3	2:B:62:ARG:HH21	1.76	0.49
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.46	0.49
2:B:21:ALA:HA	2:B:189:GLY:O	2.12	0.49
1:A:65:ASN:N	1:A:65:ASN:ND2	2.60	0.49
3:C:8:VAL:HG13	3:C:9:TYR:N	2.27	0.49
5:P:106:ASN:HD21	5:P:119:ARG:HD2	1.77	0.49
2:M:83:ASP:HB2	2:M:86:TYR:H	1.77	0.49
1:A:378:GLU:OE1	2:B:26:THR:HB	2.12	0.49
2:M:152:ARG:HH21	2:M:152:ARG:HG3	1.77	0.49
1:L:65:ASN:HA	1:L:187:LEU:HD11	1.94	0.49
2:M:36:HIS:HB3	2:M:41:TYR:CE1	2.48	0.49
1:A:112:THR:HB	1:A:213:ILE:HG21	1.93	0.49
7:G:53:ASN:HB2	7:G:54:PRO:HD2	1.93	0.49
1:A:120:ASN:ND2	1:A:124:ILE:HD12	2.21	0.49
11:V:29:ILE:HA	11:V:92:ILE:HG21	1.95	0.49
3:N:129:PHE:CD1	3:N:147:ILE:HD12	2.48	0.49
2:M:205:LEU:HD12	2:M:205:LEU:H	1.78	0.49
5:E:44:LYS:HB2	8:H:35:LYS:HE3	1.94	0.49
2:M:146:LEU:O	2:M:150:THR:HG23	2.12	0.49
12:W:94:LYS:HG3	12:W:95:ASP:N	2.27	0.49
1:A:376:LEU:HD22	1:A:388:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:42:PRO:C	10:J:44:ASN:H	2.15	0.49
10:U:37:TRP:CZ3	10:U:96:CYS:HB3	2.47	0.49
2:B:193:VAL:HG23	2:B:196:ASP:HB2	1.94	0.49
11:V:17:ASP:HB2	11:V:18:ARG:HH22	1.76	0.49
11:K:61:ARG:HB2	11:K:76:SER:HB3	1.94	0.49
9:T:48:LEU:O	9:T:52:VAL:HG23	2.13	0.49
3:N:7:ASN:ND2	3:N:9:TYR:N	2.57	0.48
1:A:129:ASN:C	1:A:131:LEU:H	2.16	0.48
3:C:108:SER:CB	3:C:109:PRO:CD	2.91	0.48
10:J:23:SER:HA	10:J:78:GLN:HB3	1.94	0.48
3:C:80:TYR:CE1	3:C:248:PRO:HB2	2.47	0.48
1:A:85:ALA:HB2	1:A:118:PHE:CE1	2.47	0.48
10:J:54:ASN:H	10:J:54:ASN:ND2	2.03	0.48
2:B:252:GLN:O	2:B:255:VAL:HG22	2.12	0.48
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.41	0.48
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.44	0.48
11:K:4:LEU:HD22	11:K:88:CYS:SG	2.53	0.48
3:N:172:SER:OG	3:N:174:PRO:HD2	2.14	0.48
8:S:56:PHE:CE2	8:S:57:LEU:HG	2.48	0.48
8:H:44:ALA:HA	8:H:47:ASN:HB3	1.94	0.48
1:L:312:ASP:OD1	1:L:334:ARG:HD3	2.13	0.48
3:N:214:GLY:O	3:N:218:ARG:HD3	2.13	0.48
11:V:6:GLN:OE1	11:V:87:PHE:HA	2.12	0.48
1:A:92:LEU:HD21	1:A:118:PHE:CE2	2.48	0.48
10:U:87:THR:HG22	10:U:88:THR:H	1.79	0.48
2:M:22:ARG:HB3	2:M:191:ASN:H	1.79	0.48
7:G:29:ALA:O	7:G:33:ILE:HG13	2.12	0.48
9:I:12:LYS:O	9:I:13:ARG:HG3	2.13	0.48
3:C:362:TYR:HA	3:C:366:ILE:HB	1.95	0.48
1:L:287:TYR:HE2	1:L:295:ARG:HG2	1.79	0.48
10:J:24:VAL:CG2	10:J:29:ILE:HD11	2.43	0.48
3:C:320:VAL:HG13	8:H:58:TYR:HE2	1.78	0.48
3:N:22:GLN:O	3:N:218:ARG:HD2	2.13	0.48
2:B:145:GLN:O	2:B:149:ILE:HG12	2.13	0.48
2:M:45:ASP:HB2	2:M:165:GLU:HG2	1.96	0.48
3:C:18:ILE:HA	3:C:222:HIS:HB2	1.95	0.48
11:V:19:VAL:HG22	11:V:20:THR:N	2.29	0.48
8:H:35:LYS:O	8:H:37:LEU:N	2.47	0.48
4:D:286:TRP:CZ3	5:E:59:MET:HG3	2.48	0.48
12:W:16:LYS:O	12:W:20:LEU:HB3	2.14	0.48
2:M:43:THR:HG22	2:M:175:PHE:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:LYS:H	2:B:347:LYS:CD	2.19	0.48
2:B:119:LEU:HA	2:B:123:VAL:HB	1.94	0.48
8:S:88:GLU:O	8:S:91:ARG:HB3	2.13	0.48
2:M:30:THR:HG23	2:M:190:GLU:HB3	1.96	0.48
3:C:7:ASN:ND2	3:C:9:TYR:N	2.61	0.47
3:N:229:ASP:O	3:N:233:VAL:HG23	2.14	0.47
11:V:37:GLN:HB2	11:V:47:LEU:HD11	1.95	0.47
2:M:225:LEU:HD21	2:M:244:PRO:CD	2.44	0.47
10:U:18:LEU:HD11	10:U:118:VAL:HG11	1.95	0.47
9:I:6:LEU:O	9:I:10:PHE:HD2	1.97	0.47
2:B:242:GLY:HA2	2:B:285:PHE:O	2.14	0.47
10:J:11:LEU:HD13	10:J:125:ARG:HD2	1.96	0.47
3:N:342:CYS:SG	8:S:70:TRP:HH2	2.36	0.47
10:J:27:TYR:HE2	10:J:32:GLY:N	2.13	0.47
2:B:175:PHE:CE2	2:B:179:VAL:HG21	2.49	0.47
10:U:4:LEU:N	10:U:4:LEU:HD12	2.30	0.47
4:D:280:LEU:HD11	5:E:66:LEU:CB	2.43	0.47
8:H:58:TYR:O	8:H:62:PRO:HG2	2.14	0.47
1:L:58:ALA:HB3	1:L:98:ARG:HA	1.97	0.47
5:E:91:MET:HG3	5:E:91:MET:O	2.14	0.47
1:A:72:TRP:CZ3	1:A:75:ILE:HD11	2.49	0.47
11:K:75:ILE:HG22	11:K:76:SER:N	2.30	0.47
2:M:146:LEU:HD13	2:M:354:VAL:HG22	1.95	0.47
2:M:298:SER:OG	2:M:363:PRO:HD3	2.14	0.47
2:B:183:GLU:HB2	2:B:212:GLY:O	2.15	0.47
5:E:187:ILE:H	5:E:187:ILE:CD1	2.13	0.47
2:M:305:VAL:HG11	2:M:368:LEU:HB3	1.95	0.47
4:D:69:LEU:HD12	4:D:217:TYR:CE2	2.49	0.47
1:L:133:SER:O	1:L:134:SER:HB2	2.15	0.47
2:B:106:ALA:HB2	2:B:206:LEU:HD22	1.97	0.47
5:E:188:SER:HB3	5:E:190:ARG:HG3	1.96	0.47
3:C:121:PHE:CZ	3:C:125:ILE:HD11	2.50	0.47
1:L:171:THR:HG23	1:L:241:ALA:HA	1.97	0.47
2:B:109:LEU:HD23	2:B:180:TYR:CD2	2.50	0.47
2:M:315:SER:HB3	2:M:344:LYS:CB	2.45	0.47
4:D:246:GLN:HA	6:F:146:LEU:HD22	1.97	0.47
3:C:64:SER:O	3:C:67:HIS:HB3	2.15	0.47
4:O:76:TRP:CE2	4:O:188:CYS:HB3	2.50	0.47
2:B:94:LEU:O	2:B:96:ASP:N	2.48	0.47
2:B:135:GLU:O	2:B:135:GLU:HG2	2.15	0.47
11:K:21:ILE:HG22	11:K:22:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:120:HIS:HD2	5:P:151:GLN:HG2	1.80	0.47
7:R:95:LYS:HB2	7:R:98:GLU:HG3	1.97	0.47
12:W:22:CYS:O	12:W:32:LYS:HB2	2.15	0.47
4:O:134:TYR:HE2	4:O:149:GLY:HA3	1.80	0.47
1:L:66:ASN:HD22	1:L:180:THR:HG23	1.80	0.47
3:C:88:PHE:O	3:C:92:VAL:HG23	2.15	0.47
10:U:21:THR:HG22	10:U:80:PHE:CD2	2.49	0.47
8:S:38:GLN:CD	8:S:39:GLY:H	2.19	0.47
7:R:98:GLU:O	7:R:100:VAL:N	2.45	0.47
2:M:24:ALA:HB1	2:M:25:PRO:HD2	1.97	0.47
11:V:88:CYS:O	11:V:98:PHE:HA	2.15	0.46
11:K:29:ILE:CA	11:K:92:ILE:HG21	2.46	0.46
3:C:80:TYR:CD1	3:C:248:PRO:HB2	2.50	0.46
4:D:93:GLY:HA3	4:D:254:PHE:HB2	1.97	0.46
10:U:38:ILE:HD11	10:U:46:LEU:HD22	1.97	0.46
3:N:110:ARG:HH11	3:N:314:ARG:NH2	2.14	0.46
2:B:251:ALA:HB1	2:B:339:ASN:HB3	1.97	0.46
12:W:40:ILE:O	12:W:64:TRP:HB2	2.15	0.46
9:I:54:ALA:C	9:I:56:ILE:H	2.19	0.46
5:E:191:ILE:HG22	5:E:199:ASN:OD1	2.14	0.46
1:L:260:ILE:CD1	1:L:343:ILE:HD11	2.42	0.46
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.51	0.46
2:B:62:ARG:CG	2:B:62:ARG:HH21	2.27	0.46
5:P:187:ILE:HD12	5:P:187:ILE:N	2.31	0.46
1:L:144:LEU:HD21	1:L:185:GLU:HB3	1.97	0.46
3:C:56:SER:HB2	3:C:177:GLN:HA	1.96	0.46
7:R:90:ARG:HG2	7:R:93:TRP:CZ2	2.51	0.46
4:D:87:HIS:HA	4:D:90:ILE:HD12	1.98	0.46
1:L:129:ASN:O	1:L:131:LEU:N	2.46	0.46
10:J:99:SER:HB3	10:J:109:MET:CG	2.44	0.46
2:B:202:ASP:C	2:B:204:SER:H	2.19	0.46
1:L:66:ASN:HD21	1:L:176:PRO:HG2	1.80	0.46
10:J:20:LEU:HD22	10:J:116:THR:HG21	1.97	0.46
1:L:369:LEU:HD13	1:L:409:ILE:HD13	1.97	0.46
10:U:49:VAL:CG1	10:U:68:LEU:HD23	2.46	0.46
2:M:35:VAL:CG1	2:M:179:VAL:HG12	2.46	0.46
3:C:212:ILE:CD1	7:G:75:ILE:HG23	2.46	0.46
2:M:313:ASP:O	2:M:314:LEU:HB2	2.15	0.46
2:B:91:ALA:O	2:B:93:PHE:HD2	1.98	0.46
3:C:41:VAL:O	3:C:45:VAL:HG23	2.16	0.46
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:OD1	1:A:396:LYS:HD2	2.16	0.46
5:P:38:ASN:HD21	5:P:40:ASP:CG	2.19	0.46
3:C:7:ASN:ND2	3:C:9:TYR:H	2.13	0.46
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.50	0.46
1:L:62:ASN:N	1:L:65:ASN:ND2	2.47	0.46
3:N:107:ARG:HB3	3:N:108:SER:H	1.54	0.46
8:S:76:TYR:CE2	8:S:80:LEU:HD11	2.51	0.46
3:N:31:ASN:ND2	3:N:229:ASP:HA	2.30	0.46
3:C:131:GLY:HA3	3:C:183:HIS:CE1	2.51	0.46
5:E:85:THR:O	5:E:88:VAL:HG22	2.16	0.46
2:B:355:ALA:HB1	2:B:362:LEU:HD23	1.97	0.46
1:L:371:LEU:HD21	2:M:77:THR:HG23	1.98	0.46
2:M:31:LEU:HB2	2:M:93:PHE:HE2	1.81	0.46
1:L:287:TYR:CE1	1:L:305:ILE:HD11	2.51	0.46
2:B:339:ASN:HA	2:B:342:ALA:CB	2.46	0.46
1:L:288:ASN:C	1:L:288:ASN:ND2	2.69	0.46
5:P:187:ILE:H	5:P:187:ILE:CD1	2.27	0.46
2:M:233:PHE:HB3	2:M:357:GLY:HA2	1.97	0.46
1:A:337:THR:HG22	8:H:15:HIS:HD2	1.81	0.46
2:M:197:LEU:O	2:M:201:VAL:HG23	2.15	0.46
5:P:146:ARG:O	5:P:202:ILE:HD13	2.16	0.46
6:F:111:GLN:HB3	6:F:112:PRO:HD2	1.96	0.46
11:K:2:ILE:N	11:K:2:ILE:HD12	2.29	0.45
2:M:83:ASP:CB	2:M:86:TYR:H	2.29	0.45
3:N:312:VAL:HG21	7:R:5:PHE:CE1	2.51	0.45
3:N:375:ASN:HB3	7:R:8:ILE:CD1	2.47	0.45
1:A:69:SER:HB3	1:A:96:ILE:HD12	1.97	0.45
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.51	0.45
2:B:315:SER:N	2:B:316:PRO:HD3	2.32	0.45
11:V:6:GLN:HB2	11:V:100:ALA:HB3	1.97	0.45
6:F:106:LYS:HA	6:F:109:GLN:HE21	1.81	0.45
5:P:126:ILE:HG21	5:P:150:PRO:HB2	1.98	0.45
3:N:42:ILE:O	3:N:46:THR:HG23	2.16	0.45
10:J:79:PHE:HD2	10:J:79:PHE:H	1.63	0.45
2:B:98:LEU:N	2:B:99:PRO:HD2	2.31	0.45
1:L:237:LEU:CD2	1:L:237:LEU:H	2.22	0.45
1:L:168:PHE:O	1:L:174:SER:HB3	2.16	0.45
2:M:34:LYS:HB3	2:M:86:TYR:HD1	1.81	0.45
2:B:228:GLU:HA	2:B:353:TYR:O	2.17	0.45
10:U:95:TYR:CE1	10:U:115:GLY:HA3	2.51	0.45
2:B:200:PHE:O	2:B:204:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:76:TYR:CE1	3:N:77:ILE:HG13	2.51	0.45
1:L:248:VAL:O	1:L:433:ALA:HA	2.16	0.45
2:B:258:ASN:ND2	2:B:324:LYS:HB3	2.32	0.45
9:T:5:SER:O	9:T:9:THR:HG23	2.17	0.45
10:U:51:TYR:C	10:U:51:TYR:CD2	2.89	0.45
3:N:57:ASN:HA	3:N:173:ASN:HD21	1.82	0.45
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.16	0.45
2:M:315:SER:N	2:M:316:PRO:HD3	2.31	0.45
9:T:52:VAL:O	9:T:56:ILE:HG12	2.16	0.45
4:D:72:PRO:HG2	4:D:74:TYR:CE2	2.51	0.45
3:N:159:ASN:N	3:N:159:ASN:HD22	2.06	0.45
1:A:171:THR:CG2	1:A:241:ALA:HA	2.46	0.45
4:D:121:THR:O	4:D:125:VAL:HG23	2.17	0.45
2:M:318:ILE:CG2	2:M:319:ASN:HD22	2.29	0.45
3:C:222:HIS:CD2	3:C:223:SER:H	2.34	0.45
4:D:187:GLY:O	4:D:191:ILE:HG12	2.17	0.45
3:C:74:ASN:OD1	5:E:77:THR:HG23	2.17	0.45
7:R:63:LEU:HA	7:R:64:PRO:HD2	1.77	0.45
5:E:44:LYS:CB	8:H:35:LYS:HE3	2.47	0.45
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.98	0.45
1:A:89:GLY:HA3	2:B:319:ASN:O	2.17	0.45
4:O:302:PHE:HB2	7:R:73:TYR:CD1	2.51	0.45
4:O:304:PRO:HA	4:O:305:PRO:HD2	1.81	0.45
10:J:54:ASN:N	10:J:54:ASN:HD22	2.05	0.45
1:L:302:LEU:O	1:L:306:GLN:HG3	2.16	0.45
10:U:41:PHE:CD2	10:U:92:ALA:HB2	2.44	0.45
3:N:125:ILE:HG22	15:N:525:SMA:H40	1.97	0.45
5:P:104:GLY:O	5:P:105:LYS:HD2	2.16	0.45
10:J:70:ILE:HG23	10:J:80:PHE:O	2.16	0.45
3:C:107:ARG:HB2	3:C:108:SER:H	1.64	0.45
3:C:208:ASN:HD22	3:C:210:LEU:N	2.14	0.45
1:A:225:LYS:HD2	1:A:225:LYS:H	1.82	0.45
1:L:348:LYS:HA	1:L:348:LYS:HE2	1.98	0.45
3:C:223:SER:O	3:C:224:TYR:CG	2.70	0.45
4:D:283:LEU:O	4:D:287:VAL:HG23	2.17	0.45
6:Q:108:GLN:HA	6:Q:111:GLN:HG3	1.98	0.44
1:A:57:GLY:H	1:A:60:ASN:ND2	2.15	0.44
1:A:91:ALA:HB3	1:A:106:SER:HB2	1.99	0.44
3:C:212:ILE:HD12	7:G:75:ILE:HG23	1.99	0.44
1:L:257:LYS:HB2	1:L:259:TRP:CH2	2.51	0.44
1:L:353:LEU:O	1:L:418:LYS:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:123:CYS:HA	6:F:126:GLU:OE1	2.17	0.44
5:P:120:HIS:CD2	5:P:151:GLN:HG2	2.51	0.44
9:T:8:LYS:O	9:T:12:LYS:HG2	2.17	0.44
2:M:252:GLN:HG3	2:M:253:TYR:N	2.31	0.44
5:E:180:CYS:SG	3:N:269:ILE:HD13	2.58	0.44
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.98	0.44
10:U:14:PRO:O	10:U:15:SER:HB3	2.17	0.44
3:C:130:LEU:HD13	3:C:182:LEU:HB3	1.98	0.44
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.47	0.44
1:L:31:GLN:NE2	1:L:393:VAL:HB	2.32	0.44
3:C:137:GLY:O	3:C:140:SER:HB2	2.18	0.44
4:D:115:LEU:HD12	4:D:257:TRP:CH2	2.52	0.44
2:B:293:ASP:OD2	2:B:295:ALA:HB3	2.17	0.44
13:C:502:HEM:HMB1	13:C:502:HEM:HBB2	1.99	0.44
3:C:269:ILE:HG23	3:C:269:ILE:O	2.18	0.44
1:A:130:LEU:C	1:A:132:SER:H	2.20	0.44
5:P:190:ARG:HH21	5:P:190:ARG:HB2	1.83	0.44
4:D:111:ALA:HA	4:D:154:TYR:HA	2.00	0.44
2:B:188:SER:OG	2:B:332:VAL:HG21	2.17	0.44
3:C:147:ILE:O	3:C:150:LEU:HB2	2.17	0.44
2:M:340:PHE:O	2:M:341:ASP:CB	2.66	0.44
2:B:35:VAL:HG12	2:B:179:VAL:HG12	2.00	0.44
10:J:51:TYR:CD2	10:J:51:TYR:C	2.90	0.44
3:N:242:LEU:HD23	3:N:242:LEU:HA	1.85	0.44
11:V:2:ILE:N	11:V:2:ILE:HD12	2.30	0.44
12:W:95:ASP:O	12:W:99:LEU:HB2	2.18	0.44
10:U:68:LEU:HA	10:U:82:LYS:O	2.17	0.44
4:O:74:TYR:CE1	6:Q:139:ALA:HA	2.53	0.44
3:C:323:LYS:HD3	8:H:55:GLN:HE22	1.82	0.44
10:U:54:ASN:N	10:U:54:ASN:ND2	2.60	0.44
1:A:129:ASN:O	1:A:130:LEU:HB2	2.18	0.44
3:C:58:ILE:HB	3:C:173:ASN:HA	2.00	0.44
2:B:69:ARG:HG2	2:B:69:ARG:HH21	1.83	0.44
2:M:250:LEU:HD23	2:M:251:ALA:N	2.32	0.44
1:A:92:LEU:HD23	1:A:105:VAL:HG22	2.00	0.44
12:W:43:ARG:HD2	12:W:47:GLN:HB2	1.99	0.44
4:O:87:HIS:HA	4:O:90:ILE:HD12	2.00	0.44
2:B:232:ARG:NH1	2:M:158:PRO:HG2	2.33	0.44
7:R:123:ILE:O	7:R:123:ILE:HG13	2.18	0.44
1:A:286:SER:HA	1:A:315:ASN:HA	1.99	0.44
2:M:242:GLY:HA2	2:M:285:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:44:HIS:O	12:W:47:GLN:HG2	2.17	0.44
5:E:134:MET:CG	10:J:31:SER:HB3	2.47	0.44
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.82	0.44
3:C:320:VAL:HG13	8:H:58:TYR:CE2	2.52	0.44
5:E:106:ASN:HD22	5:E:119:ARG:HB2	1.82	0.44
2:B:367:GLU:HG2	2:B:367:GLU:H	1.42	0.44
2:M:146:LEU:HD23	2:M:286:THR:CG2	2.47	0.44
3:N:330:VAL:O	3:N:334:VAL:HG23	2.17	0.44
1:A:127:LYS:HA	1:A:127:LYS:HD2	1.76	0.44
4:O:271:LEU:HD23	9:T:36:ILE:CG2	2.46	0.43
12:W:29:GLY:N	12:W:30:PRO:CD	2.81	0.43
11:V:15:LEU:N	11:V:15:LEU:HD12	2.33	0.43
7:G:86:HIS:HE1	8:H:47:ASN:HD21	1.65	0.43
10:U:49:VAL:HG12	10:U:68:LEU:HD23	2.00	0.43
5:E:137:LEU:HD13	5:E:190:ARG:HD3	2.00	0.43
3:C:184:TYR:CE1	13:C:501:HEM:HBC1	2.53	0.43
7:G:86:HIS:HE1	8:H:47:ASN:ND2	2.17	0.43
3:C:72:VAL:HA	5:E:85:THR:HG22	1.99	0.43
3:C:229:ASP:O	3:C:233:VAL:HG23	2.17	0.43
2:B:157:ASN:HA	2:B:158:PRO:HD3	1.90	0.43
3:C:295:MET:CE	15:C:505:SMA:H33	2.48	0.43
3:C:348:TYR:OH	8:H:74:ASN:OD1	2.36	0.43
2:M:205:LEU:O	2:M:209:LEU:HG	2.18	0.43
5:P:103:LEU:O	5:P:120:HIS:O	2.36	0.43
1:A:237:LEU:N	1:A:237:LEU:HD23	2.33	0.43
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.53	0.43
4:O:78:HIS:HB3	4:O:85:PHE:HA	2.01	0.43
1:A:85:ALA:HB1	1:A:90:LEU:HB2	2.01	0.43
3:C:110:ARG:O	3:C:113:LEU:HB3	2.18	0.43
1:L:127:LYS:HA	1:L:127:LYS:HD2	1.85	0.43
1:A:133:SER:C	1:A:135:ASN:H	2.22	0.43
3:N:17:ILE:O	3:N:17:ILE:HG22	2.18	0.43
2:M:65:LEU:HD11	2:M:69:ARG:NH2	2.34	0.43
7:G:15:ILE:HG23	7:G:21:LEU:HB3	2.00	0.43
1:A:90:LEU:HD23	1:A:105:VAL:HG11	2.00	0.43
4:D:263:HIS:CE1	4:D:267:LYS:HE3	2.53	0.43
2:M:265:SER:OG	2:M:267:LEU:HD12	2.19	0.43
1:A:109:PRO:HB3	1:A:212:ASN:HD21	1.84	0.43
2:M:222:LYS:HB3	2:M:224:PHE:CE1	2.53	0.43
2:M:181:THR:HB	2:M:212:GLY:H	1.84	0.43
3:N:38:LEU:CD1	3:N:233:VAL:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:52:VAL:O	9:I:56:ILE:HG12	2.19	0.43
2:M:93:PHE:HD1	2:M:94:LEU:O	2.01	0.43
11:K:79:GLU:HA	11:K:80:PRO:HA	1.68	0.43
4:O:288:LYS:HD3	4:O:288:LYS:C	2.39	0.43
4:D:273:THR:HG22	4:D:277:LEU:HD12	2.00	0.43
5:P:191:ILE:HD13	5:P:196:ALA:HB3	2.00	0.43
10:J:100:GLU:O	10:J:107:TYR:HA	2.18	0.43
1:L:168:PHE:O	1:L:171:THR:HB	2.18	0.43
7:G:17:LYS:O	7:G:19:PRO:HD3	2.19	0.43
10:J:7:SER:OG	10:J:21:THR:HG23	2.19	0.43
3:C:48:ILE:HD13	3:N:185:LEU:HG	2.00	0.43
8:H:30:SER:HA	8:H:31:PRO:HD3	1.91	0.43
10:J:94:TYR:CD1	10:J:94:TYR:N	2.86	0.43
2:M:270:LEU:HA	2:M:300:ASN:HD22	1.84	0.43
1:L:67:GLY:CA	1:L:179:GLY:HA3	2.48	0.43
1:L:257:LYS:HB2	1:L:259:TRP:CZ2	2.54	0.43
10:U:126:HIS:HA	10:U:127:PRO:HD2	1.90	0.43
4:O:80:GLY:HA2	4:O:81:PRO:HD2	1.81	0.43
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.53	0.43
3:C:43:GLN:CB	13:C:501:HEM:HAB	2.49	0.43
11:K:34:ASN:ND2	11:K:49:TYR:HA	2.30	0.43
1:A:171:THR:HG23	1:A:241:ALA:HA	2.00	0.43
4:O:115:LEU:HD22	4:O:115:LEU:N	2.34	0.43
3:N:271:PRO:HG2	3:N:279:TYR:CG	2.54	0.43
2:B:298:SER:OG	2:B:363:PRO:HD3	2.18	0.43
2:M:320:TYR:C	2:M:322:LYS:N	2.71	0.43
2:M:346:PHE:CE1	2:M:347:LYS:O	2.72	0.43
10:U:28:SER:O	10:U:31:SER:HB2	2.19	0.43
1:A:226:ASN:HB3	1:A:227:LEU:H	1.47	0.43
4:O:188:CYS:SG	4:O:256:ASN:OD1	2.76	0.43
3:N:154:ILE:HA	3:N:155:PRO:HD2	1.77	0.43
3:C:125:ILE:CG2	15:C:505:SMA:H37	2.44	0.42
3:C:43:GLN:HB3	13:C:501:HEM:HAB	2.01	0.42
1:A:89:GLY:HA2	2:B:320:TYR:HB2	2.01	0.42
3:C:222:HIS:CG	3:C:223:SER:N	2.87	0.42
10:J:12:VAL:O	10:J:120:VAL:HA	2.19	0.42
5:E:104:GLY:O	5:E:105:LYS:HD2	2.18	0.42
3:C:365:ILE:O	3:C:369:VAL:HG23	2.19	0.42
2:B:64:ALA:O	2:B:68:VAL:HG23	2.18	0.42
11:V:74:THR:HG22	11:V:75:ILE:N	2.33	0.42
2:M:340:PHE:C	2:M:342:ALA:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:GLN:NE2	1:L:352:ARG:HD3	2.35	0.42
2:B:206:LEU:O	2:B:209:LEU:HB2	2.19	0.42
11:V:94:PHE:HE1	11:V:96:TRP:CZ2	2.37	0.42
1:A:56:SER:O	1:A:101:GLN:HG2	2.19	0.42
10:U:42:PRO:C	10:U:44:ASN:H	2.21	0.42
2:M:53:ARG:HB3	2:M:123:VAL:HG13	2.00	0.42
12:W:13:THR:HG22	12:W:16:LYS:CE	2.46	0.42
3:N:166:TRP:CE3	3:N:170:SER:HA	2.53	0.42
10:J:6:GLU:H	10:J:114:GLN:NE2	2.15	0.42
2:B:260:LEU:O	2:B:271:ILE:HD11	2.18	0.42
3:N:193:MET:CE	3:N:196:MET:SD	3.07	0.42
1:L:181:LEU:HD23	1:L:181:LEU:O	2.19	0.42
4:O:116:VAL:HG22	4:O:125:VAL:HG21	2.02	0.42
10:U:13:GLN:O	10:U:16:GLN:HB2	2.19	0.42
5:E:57:TYR:CD1	5:E:57:TYR:N	2.86	0.42
2:M:43:THR:HG22	2:M:175:PHE:CD1	2.54	0.42
10:U:4:LEU:HA	10:U:23:SER:O	2.19	0.42
2:M:320:TYR:C	2:M:322:LYS:H	2.23	0.42
2:B:122:SER:C	2:B:125:PRO:HD2	2.39	0.42
1:L:27:ALA:O	1:L:28:GLU:HB2	2.19	0.42
4:O:283:LEU:HD21	5:P:62:ALA:HB3	2.02	0.42
1:L:225:LYS:HD2	1:L:225:LYS:H	1.84	0.42
10:J:30:THR:O	10:J:54:ASN:HB2	2.20	0.42
11:V:8:PRO:HG3	11:V:11:LEU:HD22	2.02	0.42
8:H:39:GLY:O	8:H:44:ALA:HB3	2.20	0.42
12:W:75:ASN:CG	12:W:78:LYS:HB3	2.39	0.42
3:N:23:PRO:HB2	3:N:26:ILE:HG23	2.02	0.42
10:U:20:LEU:HD21	10:U:116:THR:HG21	2.00	0.42
1:L:238:LYS:HB2	1:L:238:LYS:HE3	1.75	0.42
10:U:61:ASN:C	10:U:61:ASN:HD22	2.23	0.42
5:E:197:PRO:HG2	5:E:198:LEU:HG	2.01	0.42
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	2.02	0.42
2:B:153:LYS:NZ	2:B:153:LYS:HB3	2.34	0.42
11:K:24:ARG:HA	11:K:69:THR:O	2.19	0.42
2:B:338:LEU:C	2:B:340:PHE:H	2.22	0.42
5:E:106:ASN:HD21	5:E:119:ARG:HD2	1.84	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.80	0.42
1:L:269:VAL:O	1:L:270:ASN:CB	2.68	0.42
1:L:364:ARG:NH2	2:M:72:GLU:OE1	2.53	0.42
2:M:209:LEU:HA	2:M:210:PRO:HD3	1.92	0.42
1:L:295:ARG:HB3	1:L:306:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:40:ARG:HD3	2:M:155:LEU:CG	2.47	0.42
11:V:33:LEU:HD13	11:V:71:TYR:CD1	2.55	0.42
12:W:16:LYS:HA	12:W:20:LEU:HB2	2.01	0.42
4:O:302:PHE:HB2	7:R:73:TYR:CE1	2.55	0.42
11:K:38:GLN:HB3	11:K:85:THR:HB	2.02	0.42
4:D:133:GLU:HA	4:D:147:ARG:O	2.20	0.42
8:H:64:GLY:O	8:H:68:TYR:HB2	2.20	0.42
3:C:25:SER:OG	7:G:79:HIS:CD2	2.73	0.42
10:J:13:GLN:HA	10:J:121:SER:O	2.20	0.42
12:W:60:LYS:HD2	12:W:60:LYS:HA	1.78	0.42
5:P:55:TYR:O	5:P:59:MET:HG2	2.19	0.42
5:E:150:PRO:HD3	10:J:102:TYR:CG	2.55	0.42
3:N:38:LEU:HD11	3:N:233:VAL:HG13	2.02	0.42
5:P:143:ASP:O	5:P:147:VAL:HG22	2.19	0.42
4:O:299:LYS:HD2	5:P:39:PHE:CE2	2.54	0.42
10:U:62:PRO:O	10:U:65:LYS:HG2	2.19	0.42
1:L:288:ASN:HD22	1:L:289:ALA:N	2.18	0.42
1:A:57:GLY:N	1:A:60:ASN:HD22	2.17	0.42
12:W:37:LEU:O	12:W:107:CYS:HB2	2.20	0.42
1:A:420:TRP:CZ3	1:A:425:LEU:HD22	2.55	0.42
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.55	0.42
2:M:214:SER:OG	2:M:216:VAL:HG23	2.20	0.42
1:L:262:LEU:HD23	1:L:262:LEU:C	2.40	0.42
4:O:247:MET:HE3	4:O:247:MET:HB2	1.97	0.42
3:N:159:ASN:H	3:N:159:ASN:ND2	2.07	0.41
5:P:103:LEU:HA	5:P:120:HIS:CE1	2.55	0.41
11:K:18:ARG:O	11:K:18:ARG:HD2	2.20	0.41
5:E:160:THR:OG1	5:E:197:PRO:HD2	2.20	0.41
1:A:89:GLY:CA	2:B:319:ASN:O	2.68	0.41
10:U:51:TYR:HD2	10:U:51:TYR:C	2.22	0.41
3:N:18:ILE:HA	3:N:222:HIS:HB2	2.02	0.41
3:C:379:TYR:CE1	3:C:383:VAL:HG21	2.54	0.41
1:A:358:THR:OG1	1:A:361:GLU:HG3	2.20	0.41
2:M:68:VAL:O	2:M:72:GLU:HG3	2.20	0.41
4:O:209:PRO:O	4:O:212:SER:HB2	2.20	0.41
3:C:342:CYS:SG	8:H:70:TRP:HH2	2.43	0.41
9:T:14:ASN:HD22	9:T:14:ASN:HA	1.68	0.41
3:N:12:LEU:HD23	3:N:12:LEU:HA	1.67	0.41
3:N:108:SER:OG	3:N:109:PRO:CD	2.67	0.41
11:V:32:PHE:CD2	11:V:92:ILE:HG22	2.56	0.41
1:A:171:THR:HG21	1:A:242:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:LYS:HE3	10:J:65:LYS:HB2	1.87	0.41
12:W:87:PHE:CE1	12:W:89:GLY:HA2	2.56	0.41
7:G:31:GLN:HA	7:G:31:GLN:NE2	2.34	0.41
7:R:83:LEU:HD12	7:R:83:LEU:C	2.41	0.41
11:V:4:LEU:CD2	11:V:88:CYS:SG	3.09	0.41
3:N:319:LYS:HB2	3:N:322:SER:HB2	2.02	0.41
1:L:250:LEU:HD23	8:S:25:THR:CG2	2.50	0.41
10:J:93:THR:HB	10:J:117:THR:HG23	2.02	0.41
2:M:26:THR:OG1	2:M:191:ASN:ND2	2.52	0.41
1:L:392:GLU:O	1:L:396:LYS:HG2	2.20	0.41
8:S:48:SER:O	8:S:50:ARG:N	2.53	0.41
7:G:86:HIS:CE1	8:H:47:ASN:ND2	2.89	0.41
4:O:283:LEU:HD12	4:O:283:LEU:HA	1.90	0.41
11:V:4:LEU:HD22	11:V:88:CYS:SG	2.61	0.41
3:N:226:ILE:HA	3:N:226:ILE:HD13	1.92	0.41
8:S:35:LYS:HA	8:S:36:PRO:HD2	1.77	0.41
3:C:347:PRO:HG3	8:H:77:ASN:CB	2.49	0.41
2:B:109:LEU:HD23	2:B:180:TYR:HD2	1.86	0.41
1:A:34:ASN:HD21	1:A:223:GLU:CD	2.24	0.41
3:N:112:THR:O	3:N:116:VAL:HG23	2.21	0.41
4:O:231:ASP:OD2	4:O:244:THR:HG22	2.20	0.41
2:M:294:SER:HB3	2:M:358:ASP:HB3	2.02	0.41
4:D:134:TYR:OH	4:D:156:PRO:HD3	2.20	0.41
10:U:48:TRP:CZ2	10:U:50:GLY:HA2	2.56	0.41
2:B:291:ASP:HB3	2:B:297:VAL:HG22	2.02	0.41
1:A:129:ASN:O	1:A:131:LEU:N	2.45	0.41
1:L:36:ILE:HG22	1:L:37:VAL:H	1.86	0.41
12:W:94:LYS:HD2	12:W:98:ASP:OD2	2.20	0.41
11:K:21:ILE:HG22	11:K:22:SER:H	1.85	0.41
2:B:91:ALA:O	2:B:93:PHE:CD2	2.74	0.41
1:A:100:PHE:CD1	1:A:101:GLN:N	2.89	0.41
2:M:64:ALA:O	2:M:68:VAL:HG23	2.21	0.41
11:V:79:GLU:HA	11:V:80:PRO:HA	1.73	0.41
1:A:28:GLU:HB3	1:A:29:VAL:H	1.55	0.41
12:W:77:M3L:HM12	12:W:83:THR:O	2.20	0.41
6:F:101:CYS:O	6:F:105:VAL:HG23	2.21	0.41
1:L:92:LEU:HD23	1:L:105:VAL:HG22	2.02	0.41
1:L:155:HIS:N	1:L:156:PRO:HD2	2.36	0.41
5:E:44:LYS:HZ2	5:E:52:GLY:H	1.66	0.41
1:L:287:TYR:CE2	1:L:295:ARG:HG2	2.56	0.41
1:L:299:ILE:HB	1:L:302:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:ARG:O	4:D:96:VAL:HG23	2.21	0.41
11:K:2:ILE:HG23	11:K:26:SER:OG	2.21	0.41
10:J:41:PHE:CD2	10:J:92:ALA:HB2	2.56	0.41
4:O:85:PHE:CE1	4:O:257:TRP:HA	2.56	0.41
1:L:381:ASN:CG	1:L:383:VAL:HG22	2.41	0.41
2:M:146:LEU:HD12	2:M:146:LEU:HA	1.85	0.41
11:K:14:SER:HB3	11:K:15:LEU:H	1.74	0.41
7:G:53:ASN:ND2	7:G:56:MET:H	2.19	0.41
12:W:73:LEU:HD13	12:W:99:LEU:HD12	2.03	0.41
1:A:73:LYS:HG3	1:A:94:SER:HB3	2.01	0.41
2:B:82:LEU:HD12	2:B:87:ILE:HG12	2.03	0.41
2:M:367:GLU:H	2:M:367:GLU:HG2	1.49	0.41
1:L:251:ARG:NH1	1:L:439:GLU:HB2	2.36	0.41
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.90	0.41
1:L:88:GLU:HB3	1:L:90:LEU:HD22	2.02	0.41
2:M:301:ILE:HG23	2:M:302:LYS:N	2.36	0.41
8:H:24:ILE:H	8:H:24:ILE:HD12	1.85	0.41
2:B:83:ASP:HB2	2:B:86:TYR:N	2.18	0.41
1:L:237:LEU:C	1:L:238:LYS:HG3	2.42	0.41
3:C:253:HIS:CD2	3:C:255:ASP:HB2	2.56	0.41
2:B:315:SER:HB2	2:B:318:ILE:HG13	2.03	0.41
5:E:118:ILE:HA	5:E:153:LEU:O	2.21	0.41
2:M:165:GLU:HG3	2:M:165:GLU:O	2.19	0.41
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.92	0.41
1:A:317:PHE:HB2	1:A:319:LEU:HD13	2.03	0.41
1:L:428:GLN:HE22	9:T:13:ARG:CZ	2.33	0.40
10:J:68:LEU:HB3	10:J:83:LEU:HD13	2.02	0.40
13:O:523:HEM:HHA	13:O:523:HEM:HBA2	2.03	0.40
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.61	0.40
2:M:241:ILE:HA	2:M:352:ASN:O	2.22	0.40
1:L:368:LEU:HA	1:L:368:LEU:HD23	1.89	0.40
2:M:124:LEU:HB2	2:M:125:PRO:HD3	2.03	0.40
11:V:89:GLN:HB3	11:V:98:PHE:CD1	2.56	0.40
3:N:159:ASN:N	3:N:159:ASN:ND2	2.69	0.40
11:V:75:ILE:CG2	11:V:76:SER:H	2.33	0.40
8:H:56:PHE:O	8:H:60:LEU:HB2	2.21	0.40
4:O:175:PRO:HG3	13:O:523:HEM:HAA1	2.03	0.40
3:C:261:ASN:HA	3:C:262:PRO:HD3	1.85	0.40
6:F:81:LEU:O	6:F:85:PHE:HD1	2.05	0.40
9:I:37:THR:O	9:I:41:GLU:HG3	2.20	0.40
3:C:40:LEU:HA	3:C:40:LEU:HD12	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:71:LYS:HB3	8:S:71:LYS:HE3	1.91	0.40
1:L:276:VAL:HA	1:L:412:ILE:HD13	2.04	0.40
11:V:4:LEU:HD12	11:V:4:LEU:N	2.36	0.40
1:A:120:ASN:O	1:A:124:ILE:HB	2.21	0.40
1:A:129:ASN:C	1:A:131:LEU:N	2.74	0.40
3:N:253:HIS:CD2	3:N:255:ASP:H	2.25	0.40
8:S:61:ILE:O	8:S:65:ILE:HG13	2.22	0.40
11:K:17:ASP:HB2	11:K:18:ARG:NH2	2.33	0.40
1:L:75:ILE:CG2	1:L:139:THR:HG21	2.51	0.40
1:A:91:ALA:O	1:A:105:VAL:HA	2.21	0.40
3:N:233:VAL:O	3:N:237:MET:HG3	2.22	0.40
4:O:112:TRP:O	4:O:115:LEU:HD23	2.21	0.40
4:D:147:ARG:NH2	4:D:150:LYS:HE3	2.37	0.40
5:E:140:PRO:O	5:E:141:GLN:HG3	2.21	0.40
10:J:52:ILE:O	10:J:52:ILE:HG23	2.21	0.40
1:L:406:PHE:CD1	1:L:406:PHE:N	2.90	0.40
3:N:58:ILE:HB	3:N:173:ASN:HD22	1.87	0.40
10:U:99:SER:HA	10:U:109:MET:HA	2.02	0.40
4:O:286:TRP:CD2	8:S:37:LEU:HD12	2.56	0.40
11:V:75:ILE:CG2	11:V:76:SER:N	2.82	0.40
11:K:29:ILE:HD11	11:K:71:TYR:CE1	2.56	0.40
2:M:35:VAL:HG13	2:M:185:LEU:HB3	2.03	0.40
4:O:183:ALA:O	4:O:184:ARG:HD3	2.21	0.40
2:M:115:LYS:HA	2:M:115:LYS:HD2	1.77	0.40
2:M:21:ALA:HB1	2:M:192:VAL:O	2.21	0.40
11:V:29:ILE:HG22	11:V:92:ILE:HD12	2.02	0.40
1:L:288:ASN:HD22	1:L:290:PHE:H	1.69	0.40
2:B:152:ARG:NH2	2:B:152:ARG:HG3	2.36	0.40
10:U:49:VAL:HG12	10:U:68:LEU:CD2	2.51	0.40
5:P:126:ILE:CG2	5:P:150:PRO:HB2	2.50	0.40
11:K:38:GLN:O	11:K:84:ALA:HB1	2.21	0.40
5:P:212:VAL:HG22	5:P:213:ILE:N	2.37	0.40
3:C:349:VAL:O	3:C:353:GLN:HG3	2.21	0.40
11:V:21:ILE:HG22	11:V:22:SER:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	428/430 (100%)	374 (87%)	47 (11%)	7 (2%)	12 46
1	L	428/430 (100%)	384 (90%)	37 (9%)	7 (2%)	12 46
2	B	350/352 (99%)	286 (82%)	47 (13%)	17 (5%)	3 15
2	M	350/352 (99%)	283 (81%)	48 (14%)	19 (5%)	2 12
3	C	383/385 (100%)	357 (93%)	21 (6%)	5 (1%)	15 52
3	N	383/385 (100%)	354 (92%)	24 (6%)	5 (1%)	15 52
4	D	243/248 (98%)	222 (91%)	20 (8%)	1 (0%)	39 79
4	O	243/248 (98%)	225 (93%)	14 (6%)	4 (2%)	12 46
5	E	183/185 (99%)	161 (88%)	19 (10%)	3 (2%)	12 46
5	P	183/185 (99%)	163 (89%)	20 (11%)	0	100 100
6	F	72/74 (97%)	65 (90%)	7 (10%)	0	100 100
6	Q	72/74 (97%)	62 (86%)	10 (14%)	0	100 100
7	G	123/126 (98%)	113 (92%)	8 (6%)	2 (2%)	12 46
7	R	123/126 (98%)	120 (98%)	2 (2%)	1 (1%)	24 65
8	H	91/93 (98%)	79 (87%)	8 (9%)	4 (4%)	3 17
8	S	91/93 (98%)	73 (80%)	13 (14%)	5 (6%)	2 12
9	I	51/57 (90%)	45 (88%)	6 (12%)	0	100 100
9	T	51/57 (90%)	45 (88%)	5 (10%)	1 (2%)	9 39
10	J	125/127 (98%)	110 (88%)	11 (9%)	4 (3%)	5 25
10	U	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	7 34
11	K	105/107 (98%)	85 (81%)	14 (13%)	6 (6%)	2 11
11	V	105/107 (98%)	83 (79%)	17 (16%)	5 (5%)	3 15
12	W	105/108 (97%)	89 (85%)	14 (13%)	2 (2%)	10 41
All	All	4413/4476 (99%)	3885 (88%)	427 (10%)	101 (2%)	8 35

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
2	B	95	LYS
2	B	152	ARG
2	B	335	PRO
2	B	336	ILE
3	C	108	SER
4	D	263	HIS
8	H	93	ASN
11	K	80	PRO
1	L	34	ASN
1	L	226	ASN
2	M	203	GLU
2	M	222	LYS
2	M	311	GLY
2	M	313	ASP
2	M	338	LEU
3	N	108	SER
3	N	346	VAL
4	O	263	HIS
8	S	36	PRO
8	S	52	PHE
1	A	29	VAL
2	B	45	ASP
2	B	320	TYR
2	B	338	LEU
3	C	215	ASN
7	G	96	ALA
8	H	37	LEU
10	J	32	GLY
10	J	65	LYS
1	L	28	GLU
2	M	36	HIS
2	M	45	ASP
2	M	335	PRO
2	M	336	ILE
2	M	340	PHE
2	M	367	GLU
3	N	158	GLY
3	N	224	TYR
4	O	139	ASP
4	O	197	GLY
10	U	65	LYS

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Mol	Chain	Res	Type
11	V	68	GLY
1	A	28	GLU
1	A	44	PRO
1	A	238	LYS
2	B	22	ARG
2	B	330	GLU
2	B	367	GLU
3	C	61	ALA
3	C	155	PRO
5	E	103	LEU
8	H	36	PRO
10	J	9	ALA
10	J	108	ALA
11	K	16	GLY
11	K	81	GLU
1	L	44	PRO
2	M	23	ASP
2	M	152	ARG
2	M	315	SER
4	O	102	ALA
8	S	42	HIS
9	T	12	LYS
11	V	30	ASN
12	W	22	CYS
2	B	222	LYS
2	B	224	PHE
2	B	349	GLY
7	G	99	ASP
11	K	78	LEU
11	K	91	HIS
2	M	224	PHE
8	S	37	LEU
10	U	27	TYR
10	U	126	HIS
11	V	80	PRO
1	A	289	ALA
2	B	313	ASP
1	L	309	GLN
2	M	97	ASP
3	N	155	PRO
7	R	99	ASP
8	S	49	PHE

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Mol	Chain	Res	Type
11	V	73	LEU
2	B	21	ALA
2	B	311	GLY
3	C	224	TYR
8	H	56	PHE
1	L	29	VAL
2	M	221	PRO
11	V	16	GLY
5	E	150	PRO
11	K	68	GLY
2	M	332	VAL
1	A	36	ILE
5	E	37	PRO
12	W	81	PRO
2	M	349	GLY
2	B	332	VAL
1	L	124	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	369/369 (100%)	333 (90%)	36 (10%)	10 35
1	L	369/369 (100%)	328 (89%)	41 (11%)	8 28
2	B	301/301 (100%)	272 (90%)	29 (10%)	10 36
2	M	301/301 (100%)	269 (89%)	32 (11%)	8 30
3	C	338/338 (100%)	311 (92%)	27 (8%)	15 45
3	N	338/338 (100%)	311 (92%)	27 (8%)	15 45
4	D	202/206 (98%)	190 (94%)	12 (6%)	24 61
4	O	202/206 (98%)	193 (96%)	9 (4%)	34 72
5	E	151/151 (100%)	141 (93%)	10 (7%)	21 56
5	P	151/151 (100%)	145 (96%)	6 (4%)	38 75
6	F	67/67 (100%)	60 (90%)	7 (10%)	9 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	Q	67/67 (100%)	58 (87%)	9 (13%)	5 19
7	G	109/110 (99%)	104 (95%)	5 (5%)	33 71
7	R	109/110 (99%)	101 (93%)	8 (7%)	17 51
8	H	77/77 (100%)	70 (91%)	7 (9%)	12 39
8	S	77/77 (100%)	69 (90%)	8 (10%)	9 31
9	I	45/47 (96%)	41 (91%)	4 (9%)	12 40
9	T	45/47 (96%)	44 (98%)	1 (2%)	60 87
10	J	112/112 (100%)	99 (88%)	13 (12%)	7 26
10	U	112/112 (100%)	96 (86%)	16 (14%)	4 17
11	K	93/93 (100%)	87 (94%)	6 (6%)	21 57
11	V	93/93 (100%)	87 (94%)	6 (6%)	21 57
12	W	88/88 (100%)	76 (86%)	12 (14%)	5 19
All	All	3816/3830 (100%)	3485 (91%)	331 (9%)	13 41

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	65	ASN
1	A	71	LEU
1	A	74	ASN
1	A	93	SER
1	A	108	LEU
1	A	114	LYS
1	A	119	LEU
1	A	125	GLN
1	A	161	GLU
1	A	163	LEU
1	A	171	THR
1	A	173	LEU
1	A	181	LEU
1	A	226	ASN
1	A	229	LEU
1	A	237	LEU
1	A	240	LYS
1	A	251	ARG
1	A	260	ILE
1	A	269	VAL

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Mol	Chain	Res	Type
1	A	270	ASN
1	A	278	LYS
1	A	305	ILE
1	A	319	LEU
1	A	323	ASP
1	A	335	ASN
1	A	342	LEU
1	A	360	THR
1	A	369	LEU
1	A	372	GLN
1	A	376	LEU
1	A	384	ASN
1	A	389	LEU
1	A	425	LEU
1	A	448	ARG
2	B	17	LEU
2	B	30	THR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	81	THR
2	B	85	GLU
2	B	88	THR
2	B	98	LEU
2	B	112	THR
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	193	VAL
2	B	206	LEU
2	B	254	GLU
2	B	267	LEU
2	B	294	SER
2	B	325	ASN
2	B	330	GLU
2	B	339	ASN
2	B	340	PHE
2	B	347	LYS
2	B	348	LEU
2	B	359	VAL
2	B	361	ASN

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Mol	Chain	Res	Type
2	B	362	LEU
2	B	367	GLU
3	C	5	LYS
3	C	12	LEU
3	C	35	LEU
3	C	56	SER
3	C	57	ASN
3	C	63	SER
3	C	79	ARG
3	C	81	LEU
3	C	89	PHE
3	C	99	LYS
3	C	107	ARG
3	C	108	SER
3	C	112	THR
3	C	150	LEU
3	C	155	PRO
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	206	SER
3	C	238	LEU
3	C	247	SER
3	C	302	LEU
3	C	312	VAL
3	C	313	VAL
3	C	319	LYS
3	C	321	LEU
3	C	377	LEU
4	D	63	THR
4	D	109	ARG
4	D	113	ARG
4	D	137	GLU
4	D	141	GLN
4	D	200	ASP
4	D	244	THR
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
4	D	301	VAL
5	E	42	VAL

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Mol	Chain	Res	Type
5	E	55	TYR
5	E	73	SER
5	E	85	THR
5	E	91	MET
5	E	114	LYS
5	E	187	ILE
5	E	197	PRO
5	E	202	ILE
5	E	213	ILE
6	F	77	GLN
6	F	80	ASP
6	F	84	HIS
6	F	94	LEU
6	F	99	GLU
6	F	119	HIS
6	F	130	LEU
7	G	16	LEU
7	G	51	GLU
7	G	77	ARG
7	G	83	LEU
7	G	127	LYS
8	H	38	GLN
8	H	43	ASN
8	H	50	ARG
8	H	56	PHE
8	H	60	LEU
8	H	68	TYR
8	H	71	LYS
9	I	4	SER
9	I	13	ARG
9	I	14	ASN
9	I	30	THR
10	J	1	GLU
10	J	21	THR
10	J	30	THR
10	J	36	ASN
10	J	39	ARG
10	J	51	TYR
10	J	54	ASN
10	J	61	ASN
10	J	64	LEU
10	J	68	LEU

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Mol	Chain	Res	Type
10	J	79	PHE
10	J	93	THR
10	J	100	GLU
11	K	15	LEU
11	K	18	ARG
11	K	33	LEU
11	K	81	GLU
11	K	92	ILE
11	K	107	LYS
1	L	30	THR
1	L	46	HIS
1	L	65	ASN
1	L	90	LEU
1	L	108	LEU
1	L	113	ASP
1	L	114	LYS
1	L	119	LEU
1	L	125	GLN
1	L	149	ASP
1	L	152	ASP
1	L	171	THR
1	L	173	LEU
1	L	175	LEU
1	L	178	ARG
1	L	182	GLU
1	L	187	LEU
1	L	217	ASP
1	L	226	ASN
1	L	237	LEU
1	L	240	LYS
1	L	250	LEU
1	L	251	ARG
1	L	260	ILE
1	L	279	LEU
1	L	288	ASN
1	L	305	ILE
1	L	313	ASN
1	L	329	PHE
1	L	331	THR
1	L	342	LEU
1	L	359	ASP
1	L	360	THR

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Mol	Chain	Res	Type
1	L	364	ARG
1	L	369	LEU
1	L	376	LEU
1	L	389	LEU
1	L	394	LEU
1	L	425	LEU
1	L	446	ARG
1	L	448	ARG
2	M	31	LEU
2	M	41	TYR
2	M	43	THR
2	M	54	PHE
2	M	62	ARG
2	M	83	ASP
2	M	85	GLU
2	M	98	LEU
2	M	111	LYS
2	M	112	THR
2	M	128	ARG
2	M	144	ASP
2	M	146	LEU
2	M	150	THR
2	M	152	ARG
2	M	166	ARG
2	M	169	LEU
2	M	193	VAL
2	M	213	LYS
2	M	215	LEU
2	M	216	VAL
2	M	250	LEU
2	M	252	GLN
2	M	266	GLU
2	M	287	LEU
2	M	318	ILE
2	M	330	GLU
2	M	339	ASN
2	M	345	ASP
2	M	347	LYS
2	M	360	SER
2	M	367	GLU
3	N	5	LYS
3	N	12	LEU

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Mol	Chain	Res	Type
3	N	17	ILE
3	N	34	SER
3	N	35	LEU
3	N	38	LEU
3	N	57	ASN
3	N	79	ARG
3	N	81	LEU
3	N	89	PHE
3	N	99	LYS
3	N	112	THR
3	N	129	PHE
3	N	150	LEU
3	N	159	ASN
3	N	175	THR
3	N	182	LEU
3	N	184	TYR
3	N	185	LEU
3	N	206	SER
3	N	208	ASN
3	N	282	LEU
3	N	312	VAL
3	N	313	VAL
3	N	317	THR
3	N	350	LEU
3	N	382	ARG
4	O	69	LEU
4	O	77	SER
4	O	83	GLU
4	O	109	ARG
4	O	113	ARG
4	O	244	THR
4	O	251	VAL
4	O	256	ASN
4	O	280	LEU
5	P	107	VAL
5	P	114	LYS
5	P	187	ILE
5	P	190	ARG
5	P	208	ASP
5	P	211	LYS
6	Q	74	ASP
6	Q	77	GLN

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Mol	Chain	Res	Type
6	Q	80	ASP
6	Q	86	LYS
6	Q	94	LEU
6	Q	116	ASP
6	Q	118	GLU
6	Q	119	HIS
6	Q	130	LEU
7	R	16	LEU
7	R	31	GLN
7	R	41	LEU
7	R	66	ASP
7	R	77	ARG
7	R	81	THR
7	R	83	LEU
7	R	97	GLN
8	S	38	GLN
8	S	42	HIS
8	S	47	ASN
8	S	50	ARG
8	S	56	PHE
8	S	60	LEU
8	S	68	TYR
8	S	71	LYS
9	T	13	ARG
10	U	5	GLN
10	U	36	ASN
10	U	38	ILE
10	U	39	ARG
10	U	51	TYR
10	U	54	ASN
10	U	57	ASP
10	U	61	ASN
10	U	66	ASP
10	U	68	LEU
10	U	79	PHE
10	U	87	THR
10	U	99	SER
10	U	124	TRP
10	U	125	ARG
10	U	126	HIS
11	V	18	ARG
11	V	33	LEU

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Mol	Chain	Res	Type
11	V	53	ARG
11	V	74	THR
11	V	92	ILE
11	V	107	LYS
12	W	10	LYS
12	W	14	LEU
12	W	21	GLN
12	W	26	GLU
12	W	36	ASN
12	W	75	ASN
12	W	78	LYS
12	W	80	ILE
12	W	93	GLU
12	W	94	LYS
12	W	99	LEU
12	W	107	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	60	ASN
1	A	65	ASN
1	A	66	ASN
1	A	120	ASN
1	A	121	GLN
1	A	126	GLN
1	A	155	HIS
1	A	199	HIS
1	A	282	GLN
1	A	288	ASN
1	A	304	ASN
1	A	309	GLN
1	A	316	HIS
1	A	335	ASN
1	A	344	HIS
1	A	387	ASN
1	A	437	GLN
2	B	49	HIS
2	B	52	ASN
2	B	191	ASN
2	B	246	ASN

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Mol	Chain	Res	Type
2	B	252	GLN
2	B	258	ASN
2	B	325	ASN
3	C	7	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	173	ASN
3	C	202	HIS
3	C	204	HIS
3	C	208	ASN
3	C	222	HIS
3	C	253	HIS
3	C	332	ASN
4	D	78	HIS
4	D	213	ASN
4	D	303	ASN
5	E	38	ASN
5	E	106	ASN
6	F	77	GLN
6	F	109	GLN
7	G	30	ASN
7	G	31	GLN
7	G	53	ASN
7	G	79	HIS
7	G	86	HIS
8	H	15	HIS
8	H	42	HIS
8	H	77	ASN
9	I	14	ASN
9	I	29	GLN
10	J	36	ASN
10	J	54	ASN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	34	ASN
11	K	89	GLN
11	K	90	HIS
11	K	91	HIS

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Mol	Chain	Res	Type
1	L	60	ASN
1	L	65	ASN
1	L	66	ASN
1	L	95	ASN
1	L	101	GLN
1	L	120	ASN
1	L	155	HIS
1	L	170	ASN
1	L	199	HIS
1	L	204	ASN
1	L	288	ASN
1	L	313	ASN
1	L	316	HIS
1	L	335	ASN
1	L	349	GLN
1	L	384	ASN
1	L	387	ASN
1	L	428	GLN
2	M	49	HIS
2	M	52	ASN
2	M	55	ASN
2	M	60	ASN
2	M	170	GLN
2	M	191	ASN
2	M	246	ASN
2	M	252	GLN
2	M	258	ASN
2	M	319	ASN
2	M	328	GLN
2	M	339	ASN
2	M	361	ASN
3	N	7	ASN
3	N	14	ASN
3	N	22	GLN
3	N	31	ASN
3	N	43	GLN
3	N	159	ASN
3	N	173	ASN
3	N	202	HIS
3	N	208	ASN
3	N	222	HIS
3	N	253	HIS

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Mol	Chain	Res	Type
3	N	332	ASN
4	O	67	HIS
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	169	ASN
4	O	256	ASN
5	P	38	ASN
5	P	97	ASN
5	P	106	ASN
5	P	184	HIS
6	Q	77	GLN
7	R	31	GLN
7	R	34	ASN
7	R	79	HIS
8	S	15	HIS
9	T	14	ASN
9	T	29	GLN
10	U	16	GLN
10	U	36	ASN
10	U	54	ASN
10	U	59	ASN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
10	U	114	GLN
11	V	31	ASN
11	V	34	ASN
11	V	91	HIS
12	W	57	ASN
12	W	61	ASN
12	W	67	ASN
12	W	75	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	M3L	W	77	12	10,11,12	0.61	0	12,14,16	1.19	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	M3L	W	77	12	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	W	77	M3L	CM3-NZ-CM2	-2.86	101.61	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	W	77	M3L	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	HEM	C	501	3	30,50,50	3.22	10 (33%)	24,82,82	2.39	10 (41%)
13	HEM	C	502	3	30,50,50	3.06	10 (33%)	24,82,82	2.44	9 (37%)
15	SMA	C	505	-	35,38,38	1.89	6 (17%)	40,52,52	2.14	12 (30%)
13	HEM	D	503	4	30,50,50	2.75	10 (33%)	24,82,82	3.69	11 (45%)
14	FES	E	504	5	0,4,4	0.00	-	0,4,4	0.00	-
13	HEM	N	521	3	30,50,50	3.09	10 (33%)	24,82,82	2.09	8 (33%)
13	HEM	N	522	3	30,50,50	2.66	10 (33%)	24,82,82	2.47	8 (33%)
15	SMA	N	525	-	35,38,38	1.91	7 (20%)	40,52,52	2.21	12 (30%)
13	HEM	O	523	4	30,50,50	2.77	8 (26%)	24,82,82	3.41	11 (45%)
14	FES	P	524	5	0,4,4	0.00	-	0,4,4	0.00	-
13	HEM	W	526	12	30,50,50	2.86	13 (43%)	24,82,82	3.66	8 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEM	C	501	3	-	0/10/54/54	0/0/8/8
13	HEM	C	502	3	-	0/10/54/54	0/0/8/8
15	SMA	C	505	-	2/2/5/10	0/33/34/34	0/2/2/2
13	HEM	D	503	4	-	0/10/54/54	0/0/8/8
14	FES	E	504	5	-	0/0/4/4	0/1/1/1
13	HEM	N	521	3	-	0/10/54/54	0/0/8/8
13	HEM	N	522	3	-	0/10/54/54	0/0/8/8
15	SMA	N	525	-	2/2/5/10	0/33/34/34	0/2/2/2
13	HEM	O	523	4	-	0/10/54/54	0/0/8/8
14	FES	P	524	5	-	0/0/4/4	0/1/1/1
13	HEM	W	526	12	-	0/10/54/54	0/0/8/8

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	503	HEM	C3B-C4B	-8.53	1.44	1.51
13	C	502	HEM	C3B-C4B	-8.40	1.44	1.51
13	W	526	HEM	C3B-C4B	-8.34	1.44	1.51
13	C	501	HEM	C3B-C4B	-8.33	1.44	1.51
13	O	523	HEM	C3B-C4B	-8.17	1.44	1.51
13	C	501	HEM	C3B-CAB	-8.10	1.36	1.51
13	N	521	HEM	C3C-CAC	-7.57	1.37	1.51
13	N	521	HEM	C3B-C4B	-7.33	1.45	1.51
13	N	521	HEM	C3B-CAB	-7.04	1.38	1.51
13	C	502	HEM	C3C-CAC	-6.81	1.38	1.51
13	C	502	HEM	C2D-C3D	-6.57	1.34	1.54
13	C	501	HEM	C3C-CAC	-6.53	1.39	1.51
13	C	501	HEM	C2D-C3D	-6.51	1.35	1.54
13	N	522	HEM	C2D-C3D	-6.43	1.35	1.54
13	N	521	HEM	C2D-C3D	-6.42	1.35	1.54
13	D	503	HEM	C2D-C3D	-6.42	1.35	1.54
13	O	523	HEM	C2D-C3D	-6.34	1.35	1.54
13	N	522	HEM	C3B-C4B	-6.14	1.46	1.51
13	W	526	HEM	C2D-C3D	-6.10	1.36	1.54
13	N	522	HEM	C3C-CAC	-5.96	1.40	1.51
13	C	502	HEM	C3B-CAB	-5.87	1.40	1.51
13	O	523	HEM	C3D-C4D	-5.77	1.44	1.51
13	C	501	HEM	C3D-C4D	-5.62	1.44	1.51
13	N	521	HEM	C3D-C4D	-5.61	1.44	1.51
13	D	503	HEM	C3D-C4D	-5.41	1.44	1.51
13	W	526	HEM	C3D-C4D	-5.19	1.44	1.51
13	C	502	HEM	C3D-C4D	-5.17	1.44	1.51
13	N	522	HEM	C3B-CAB	-4.99	1.42	1.51
13	N	522	HEM	C3D-C4D	-4.84	1.45	1.51
13	O	523	HEM	C2C-C1C	-4.48	1.44	1.52
13	W	526	HEM	C2C-C1C	-4.45	1.44	1.52
15	C	505	SMA	C3-C2	-4.34	1.34	1.39
13	C	502	HEM	C2C-C1C	-4.27	1.44	1.52
13	D	503	HEM	C2C-C1C	-3.96	1.45	1.52
13	N	522	HEM	C2C-C1C	-3.84	1.45	1.52
13	C	501	HEM	C2C-C1C	-3.68	1.45	1.52
13	O	523	HEM	CAA-C2A	-3.63	1.45	1.52
13	N	521	HEM	C2C-C1C	-3.47	1.46	1.52
15	N	525	SMA	C3-C2	-3.40	1.35	1.39
13	C	501	HEM	C2B-C1B	-2.51	1.43	1.51
13	W	526	HEM	CAD-C3D	-2.50	1.49	1.54
13	C	502	HEM	C2D-C1D	-2.38	1.44	1.51
13	O	523	HEM	C2B-C1B	-2.36	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	503	HEM	CAA-C2A	-2.32	1.48	1.52
13	C	502	HEM	C2B-C1B	-2.31	1.44	1.51
13	D	503	HEM	C2B-C1B	-2.29	1.44	1.51
13	N	521	HEM	C2D-C1D	-2.29	1.44	1.51
13	N	521	HEM	C2B-C1B	-2.26	1.44	1.51
13	W	526	HEM	C2D-C1D	-2.24	1.44	1.51
13	C	501	HEM	C2D-C1D	-2.16	1.44	1.51
13	D	503	HEM	C2D-C1D	-2.14	1.44	1.51
13	N	522	HEM	C2D-C1D	-2.12	1.44	1.51
13	N	522	HEM	C2B-C1B	-2.05	1.45	1.51
13	W	526	HEM	C2B-C1B	-2.03	1.45	1.51
13	N	521	HEM	CBC-CAC	2.05	1.41	1.29
13	W	526	HEM	C4C-NC	2.11	1.38	1.36
15	C	505	SMA	O7-C7	2.20	1.40	1.37
13	D	503	HEM	C1C-NC	2.21	1.38	1.36
15	N	525	SMA	O7-C7	2.23	1.40	1.37
13	W	526	HEM	C1C-NC	2.45	1.39	1.36
13	C	501	HEM	CBC-CAC	2.50	1.43	1.29
13	C	502	HEM	CBC-CAC	2.53	1.43	1.29
13	N	522	HEM	CBC-CAC	2.57	1.44	1.29
13	N	522	HEM	CBB-CAB	2.61	1.44	1.29
13	N	521	HEM	CBB-CAB	2.65	1.44	1.29
13	W	526	HEM	C3B-CAB	2.74	1.56	1.51
13	C	501	HEM	CBB-CAB	2.83	1.45	1.29
13	C	502	HEM	CBB-CAB	2.86	1.45	1.29
13	W	526	HEM	FE-NC	2.93	2.07	1.95
15	N	525	SMA	O1-C8A	2.94	1.41	1.36
15	C	505	SMA	C13-C12	3.03	1.62	1.54
15	N	525	SMA	C13-C12	3.07	1.62	1.54
13	O	523	HEM	CBB-CAB	3.87	1.51	1.29
13	D	503	HEM	CBC-CAC	3.91	1.51	1.29
13	O	523	HEM	CBC-CAC	4.05	1.52	1.29
13	D	503	HEM	CBB-CAB	4.09	1.52	1.29
13	W	526	HEM	CBB-CAB	4.16	1.53	1.29
15	C	505	SMA	O1-C2	4.20	1.40	1.35
13	W	526	HEM	CBC-CAC	4.31	1.54	1.29
15	N	525	SMA	O1-C2	4.74	1.40	1.35
15	C	505	SMA	C4-C4A	4.74	1.47	1.41
15	N	525	SMA	C4-C4A	4.75	1.47	1.41
15	C	505	SMA	C4A-C8A	5.06	1.47	1.41
15	N	525	SMA	C4A-C8A	5.12	1.47	1.41

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	503	HEM	C3C-CAC-CBC	-11.39	106.99	124.46
13	O	523	HEM	C3C-CAC-CBC	-11.35	107.05	124.46
13	W	526	HEM	C3C-CAC-CBC	-10.29	108.67	124.46
13	W	526	HEM	C3B-CAB-CBB	-9.40	110.04	124.46
13	D	503	HEM	C3B-CAB-CBB	-8.42	111.54	124.46
13	O	523	HEM	C3B-CAB-CBB	-6.57	114.38	124.46
15	N	525	SMA	C26-C19-C18	-6.29	107.62	118.10
15	C	505	SMA	C26-C19-C18	-6.06	108.02	118.10
13	C	501	HEM	C3B-CAB-CBB	-5.45	116.09	124.46
13	D	503	HEM	CAA-C2A-C1A	-4.07	122.59	127.01
15	N	525	SMA	C3-C4-C4A	-3.65	116.30	121.35
15	C	505	SMA	C3-C4-C4A	-3.60	116.36	121.35
13	C	501	HEM	CMA-C3A-C4A	-3.58	122.43	128.36
13	N	521	HEM	C3C-CAC-CBC	-3.43	119.20	124.46
13	D	503	HEM	CMA-C3A-C4A	-3.31	122.89	128.36
15	N	525	SMA	O7-C7-C6	-3.09	118.93	124.21
13	N	521	HEM	CMA-C3A-C4A	-3.04	123.34	128.36
13	C	502	HEM	CAA-C2A-C3A	-2.83	120.93	129.00
15	C	505	SMA	O1-C8A-C4A	-2.70	118.36	121.15
13	N	522	HEM	CMA-C3A-C4A	-2.68	123.93	128.36
15	C	505	SMA	C11-C12-C13	-2.66	108.51	114.36
15	C	505	SMA	O7-C7-C6	-2.59	119.79	124.21
13	C	501	HEM	CBA-CAA-C2A	-2.55	107.97	112.53
15	N	525	SMA	C11-C12-C13	-2.50	108.87	114.36
15	N	525	SMA	O1-C8A-C4A	-2.45	118.62	121.15
13	O	523	HEM	CAA-C2A-C3A	-2.11	122.98	129.00
13	C	502	HEM	CBA-CAA-C2A	-2.11	108.75	112.53
13	O	523	HEM	CBA-CAA-C2A	-2.05	108.85	112.53
15	C	505	SMA	O12-C12-C11	2.11	111.32	107.86
15	C	505	SMA	C18-C19-C20	2.17	125.99	118.92
13	N	521	HEM	CMA-C3A-C2A	2.18	129.80	125.24
15	N	525	SMA	O12-C12-C11	2.21	111.47	107.86
13	D	503	HEM	CMD-C2D-C3D	2.25	124.29	114.35
13	N	522	HEM	CAA-C2A-C1A	2.25	129.45	127.01
13	D	503	HEM	CMA-C3A-C2A	2.32	130.09	125.24
15	N	525	SMA	C18-C19-C20	2.40	126.74	118.92
13	O	523	HEM	CMD-C2D-C3D	2.53	125.55	114.35
13	C	501	HEM	CMD-C2D-C3D	2.54	125.59	114.35
13	N	521	HEM	CMD-C2D-C3D	2.55	125.61	114.35
13	C	501	HEM	CMA-C3A-C2A	2.59	130.66	125.24
13	O	523	HEM	CAA-C2A-C1A	2.60	129.83	127.01
13	C	501	HEM	CMC-C2C-C3C	2.82	123.56	116.53
13	N	522	HEM	CMD-C2D-C3D	2.83	126.88	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	501	HEM	CMB-C2B-C3B	2.98	123.96	116.53
13	W	526	HEM	CAD-C3D-C4D	3.02	123.12	112.47
13	D	503	HEM	C2D-C3D-C4D	3.09	106.74	101.50
13	O	523	HEM	C2D-C3D-C4D	3.10	106.75	101.50
15	C	505	SMA	C4-C3-C2	3.11	122.25	117.73
13	N	522	HEM	C2D-C3D-C4D	3.11	106.77	101.50
15	N	525	SMA	C4-C3-C2	3.14	122.29	117.73
13	O	523	HEM	CAD-C3D-C4D	3.16	123.61	112.47
15	N	525	SMA	O12-C12-C13	3.16	113.15	107.94
13	C	502	HEM	CMD-C2D-C3D	3.17	128.36	114.35
13	C	502	HEM	C2D-C3D-C4D	3.18	106.89	101.50
13	W	526	HEM	CMD-C2D-C3D	3.21	128.55	114.35
13	N	521	HEM	C2D-C3D-C4D	3.22	106.96	101.50
15	C	505	SMA	O7-C7-C8	3.36	117.85	114.47
13	C	501	HEM	C2D-C3D-C4D	3.39	107.24	101.50
13	O	523	HEM	CMB-C2B-C3B	3.40	125.02	116.53
13	O	523	HEM	CMC-C2C-C3C	3.43	125.09	116.53
13	W	526	HEM	C2D-C3D-C4D	3.59	107.58	101.50
15	C	505	SMA	O12-C12-C13	3.62	113.91	107.94
13	N	521	HEM	CAD-C3D-C2D	3.70	123.86	113.22
13	C	502	HEM	CAD-C3D-C4D	3.75	125.69	112.47
13	C	501	HEM	CAD-C3D-C4D	4.08	126.87	112.47
13	D	503	HEM	CMB-C2B-C3B	4.17	126.93	116.53
13	N	522	HEM	CAD-C3D-C2D	4.20	125.30	113.22
13	N	521	HEM	CMB-C2B-C3B	4.21	127.03	116.53
13	D	503	HEM	CMC-C2C-C3C	4.21	127.05	116.53
13	D	503	HEM	CAD-C3D-C4D	4.24	127.41	112.47
15	N	525	SMA	O7-C7-C8	4.28	118.77	114.47
13	D	503	HEM	CAD-C3D-C2D	4.33	125.68	113.22
13	N	522	HEM	CAD-C3D-C4D	4.35	127.80	112.47
13	C	502	HEM	CMC-C2C-C3C	4.36	127.41	116.53
15	C	505	SMA	O14-C14-C15	4.37	128.38	110.93
13	C	501	HEM	CAD-C3D-C2D	4.40	125.88	113.22
13	C	502	HEM	CAA-C2A-C1A	4.47	131.87	127.01
15	N	525	SMA	O14-C14-C13	4.52	119.00	108.09
15	N	525	SMA	O14-C14-C15	4.54	129.06	110.93
13	W	526	HEM	CMB-C2B-C3B	4.70	128.27	116.53
15	C	505	SMA	O14-C14-C13	4.71	119.46	108.09
13	N	521	HEM	CAD-C3D-C4D	4.73	129.14	112.47
13	C	502	HEM	CAD-C3D-C2D	4.90	127.31	113.22
13	W	526	HEM	CMC-C2C-C3C	4.93	128.84	116.53
13	C	502	HEM	CMB-C2B-C3B	5.05	129.13	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	N	522	HEM	CMC-C2C-C3C	5.44	130.10	116.53
13	W	526	HEM	CAD-C3D-C2D	5.56	129.19	113.22
13	O	523	HEM	CAD-C3D-C2D	5.68	129.55	113.22
13	N	522	HEM	CMB-C2B-C3B	5.92	131.31	116.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	N	525	SMA	C12
15	N	525	SMA	C14
15	C	505	SMA	C12
15	C	505	SMA	C14

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	501	HEM	6	0
13	C	502	HEM	1	0
15	C	505	SMA	4	0
14	E	504	FES	1	0
13	N	521	HEM	1	0
13	N	522	HEM	2	0
15	N	525	SMA	4	0
13	O	523	HEM	3	0
13	W	526	HEM	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.